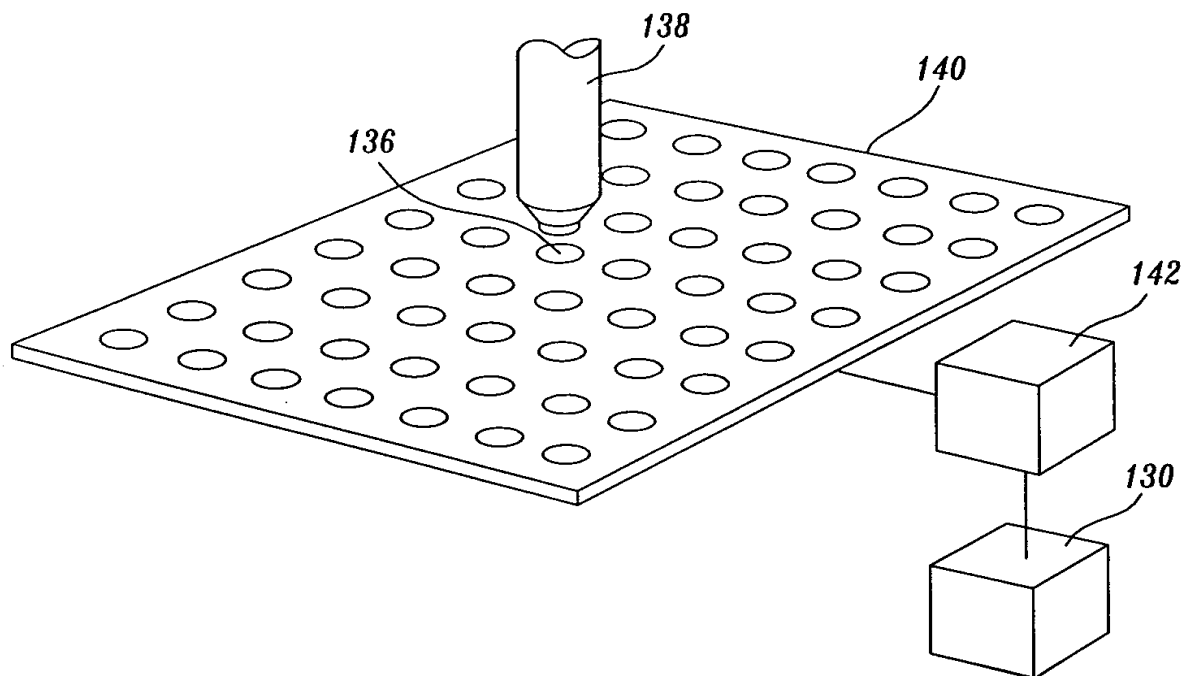


Fig. 1



*Fig. 1A.*

002080-587766  
03631185-080200

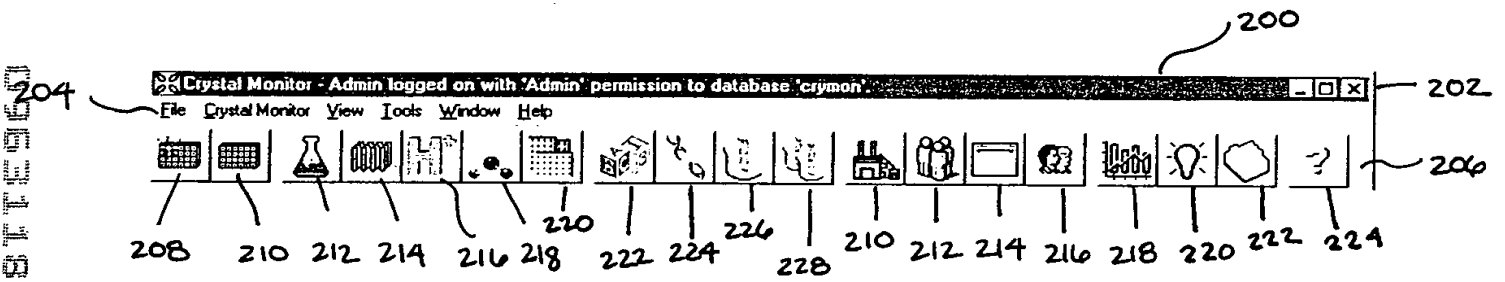


Fig. 2

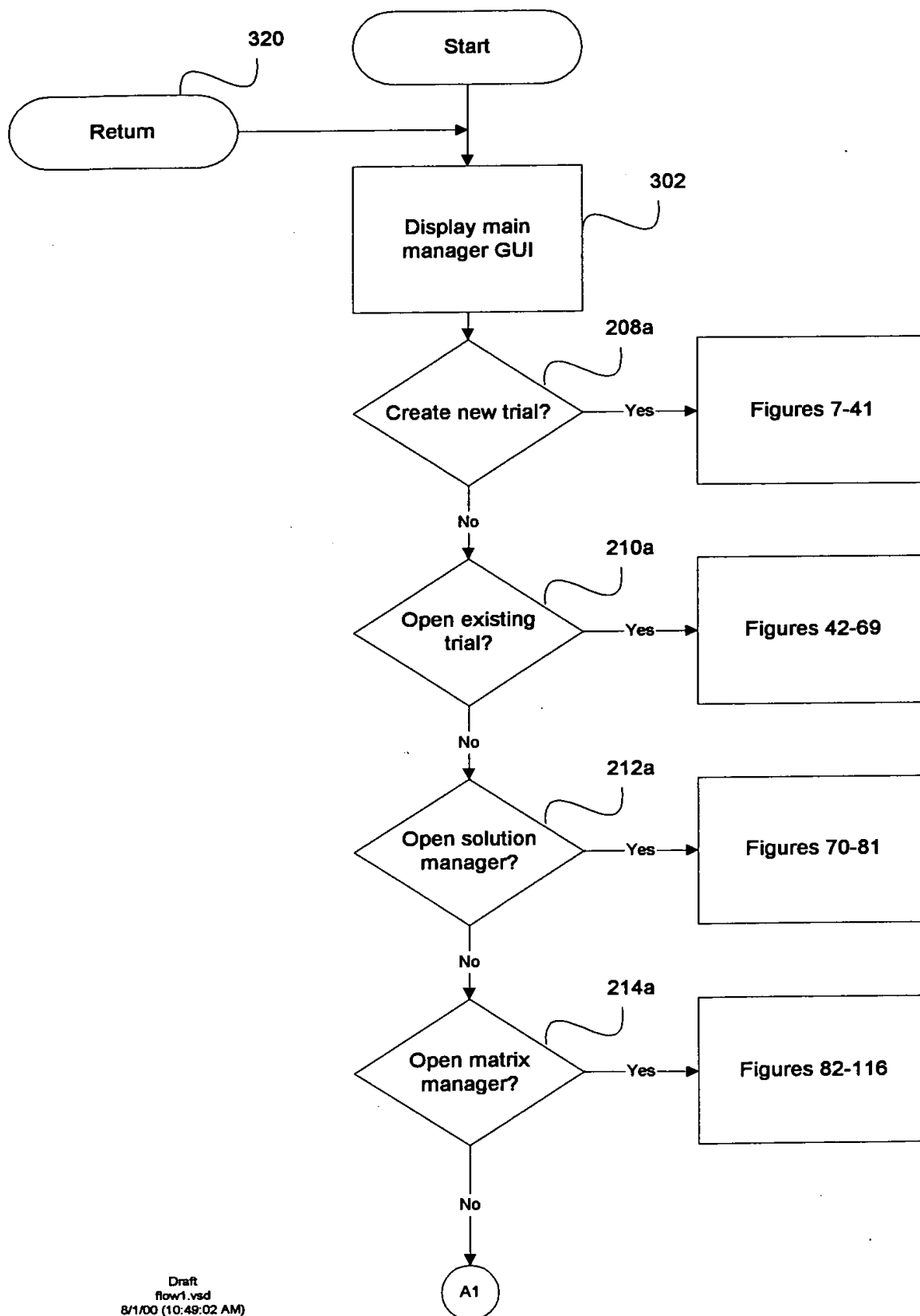


FIGURE 3

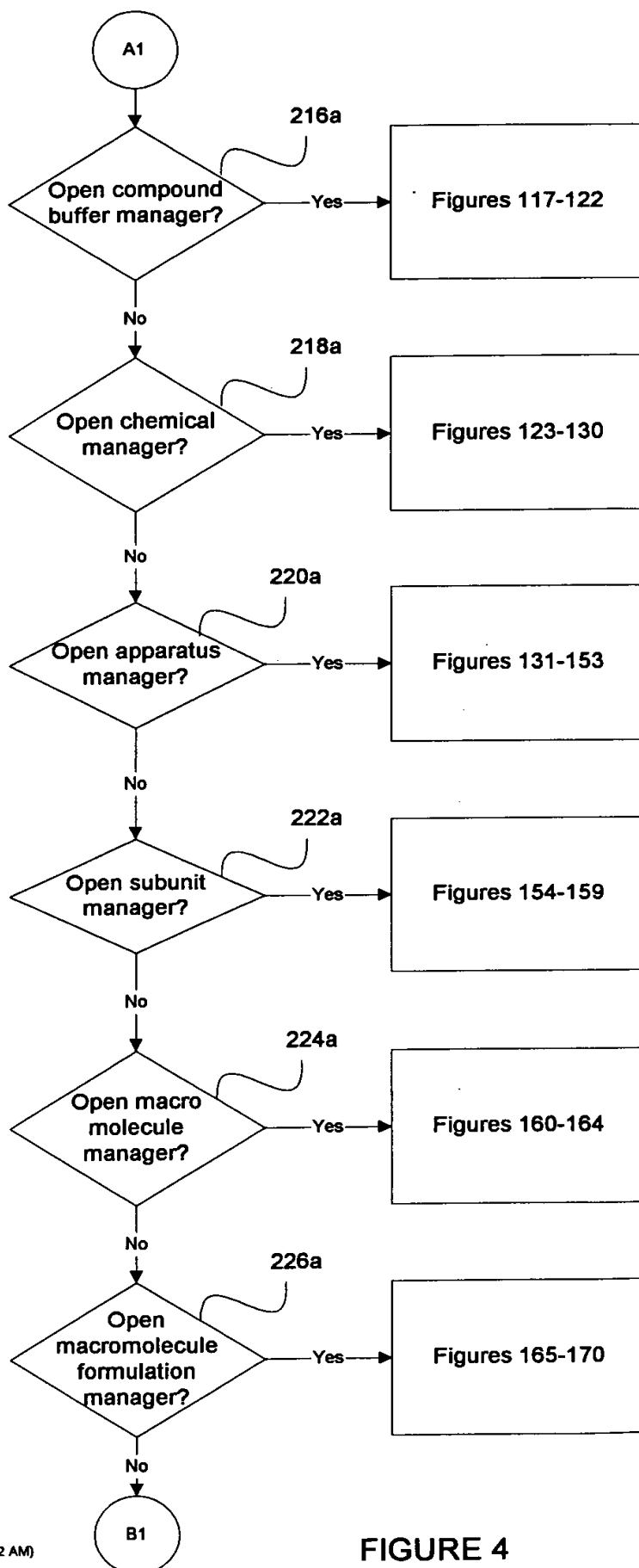


FIGURE 4

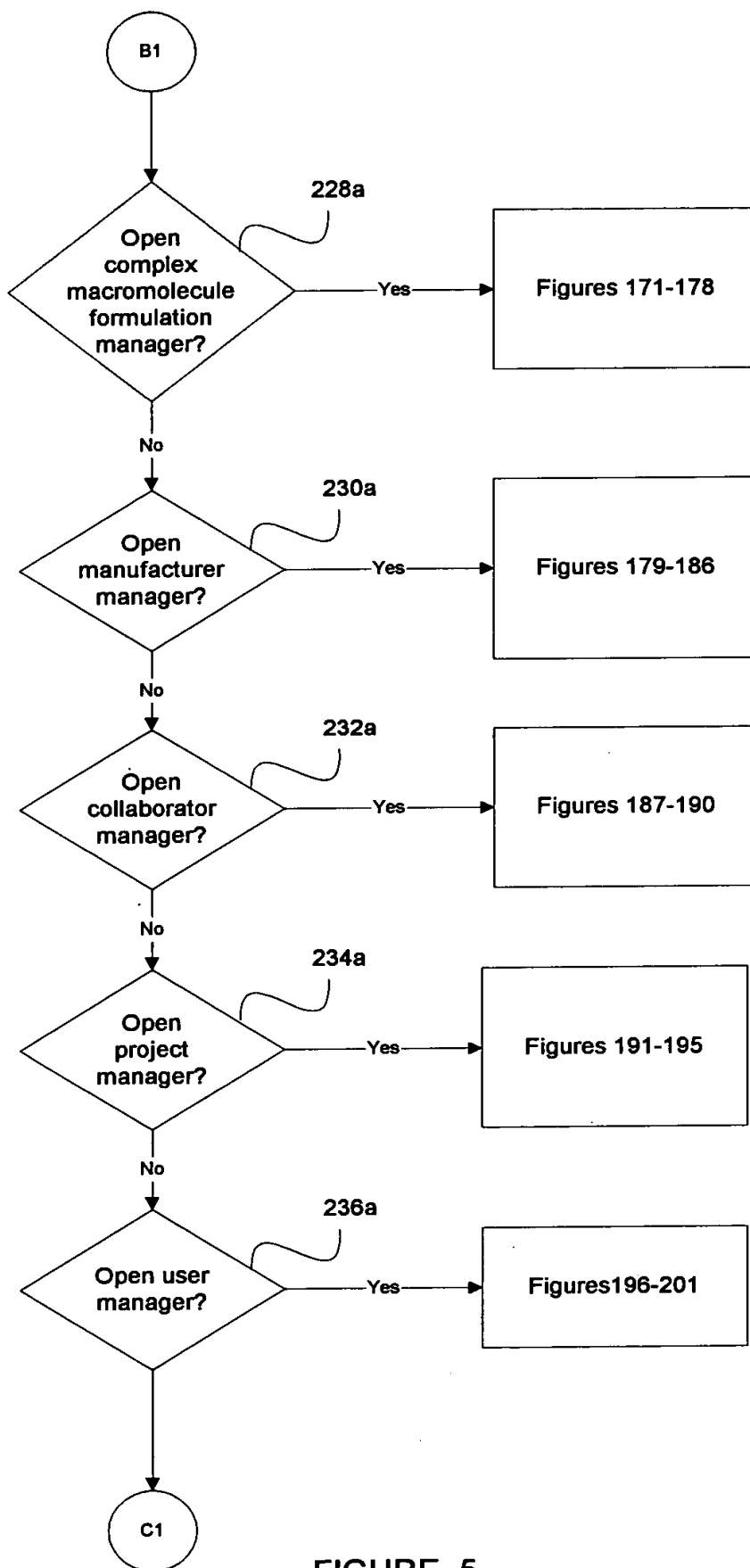


FIGURE 5

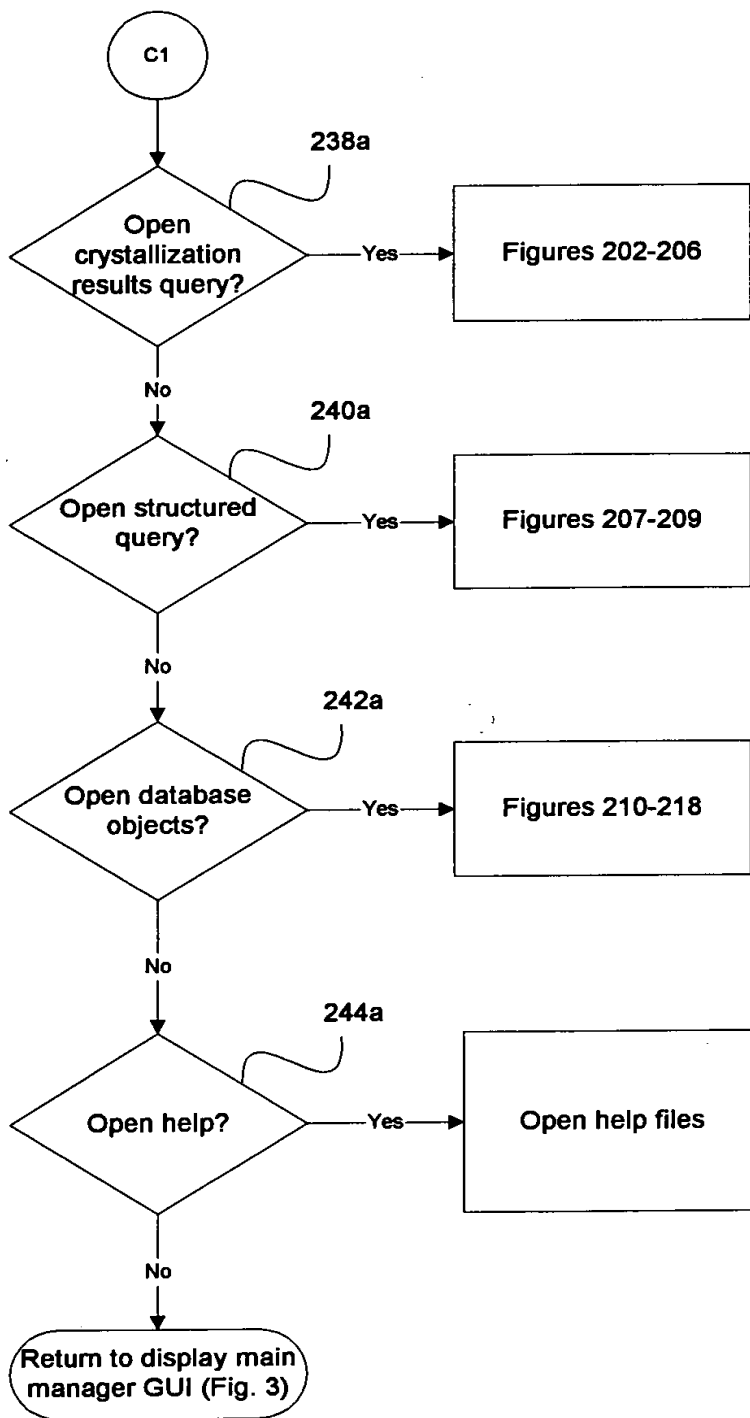
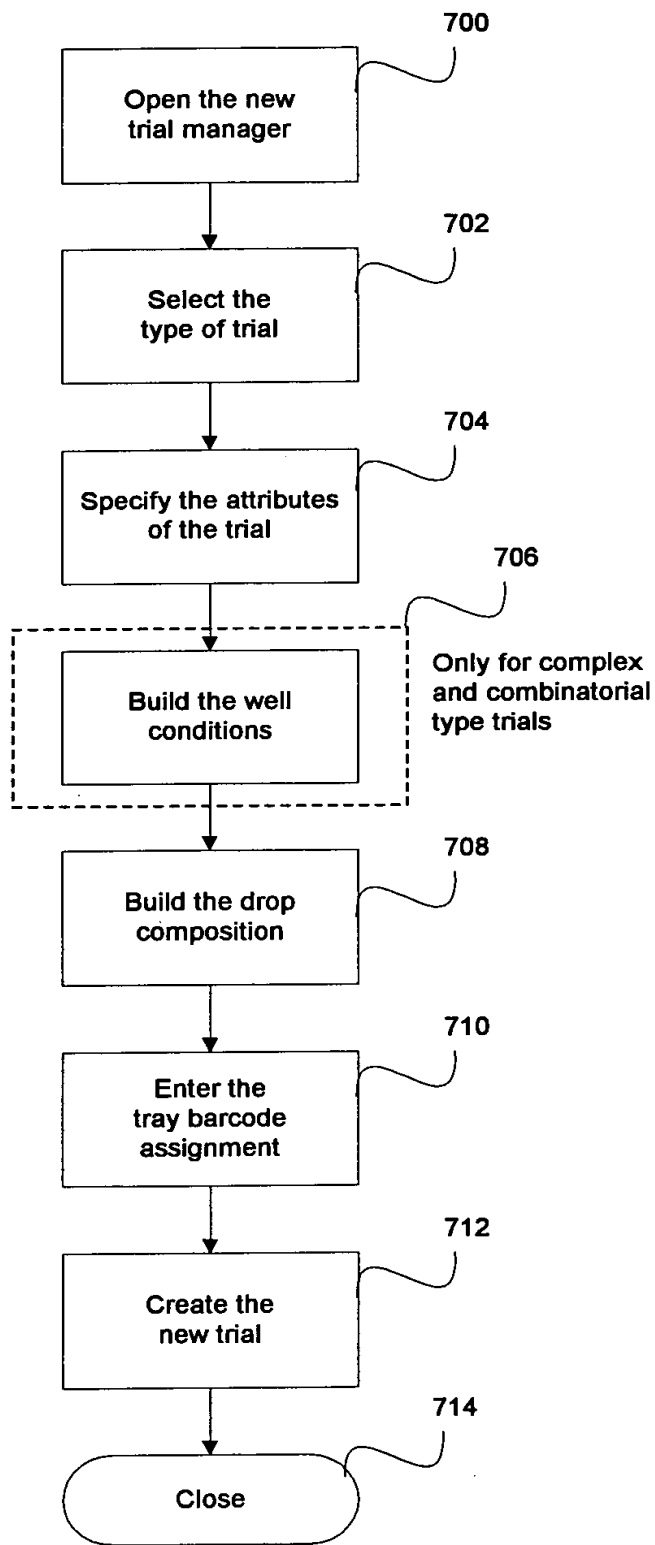


FIGURE 6



**FIGURE 7**



002080"59TTE960

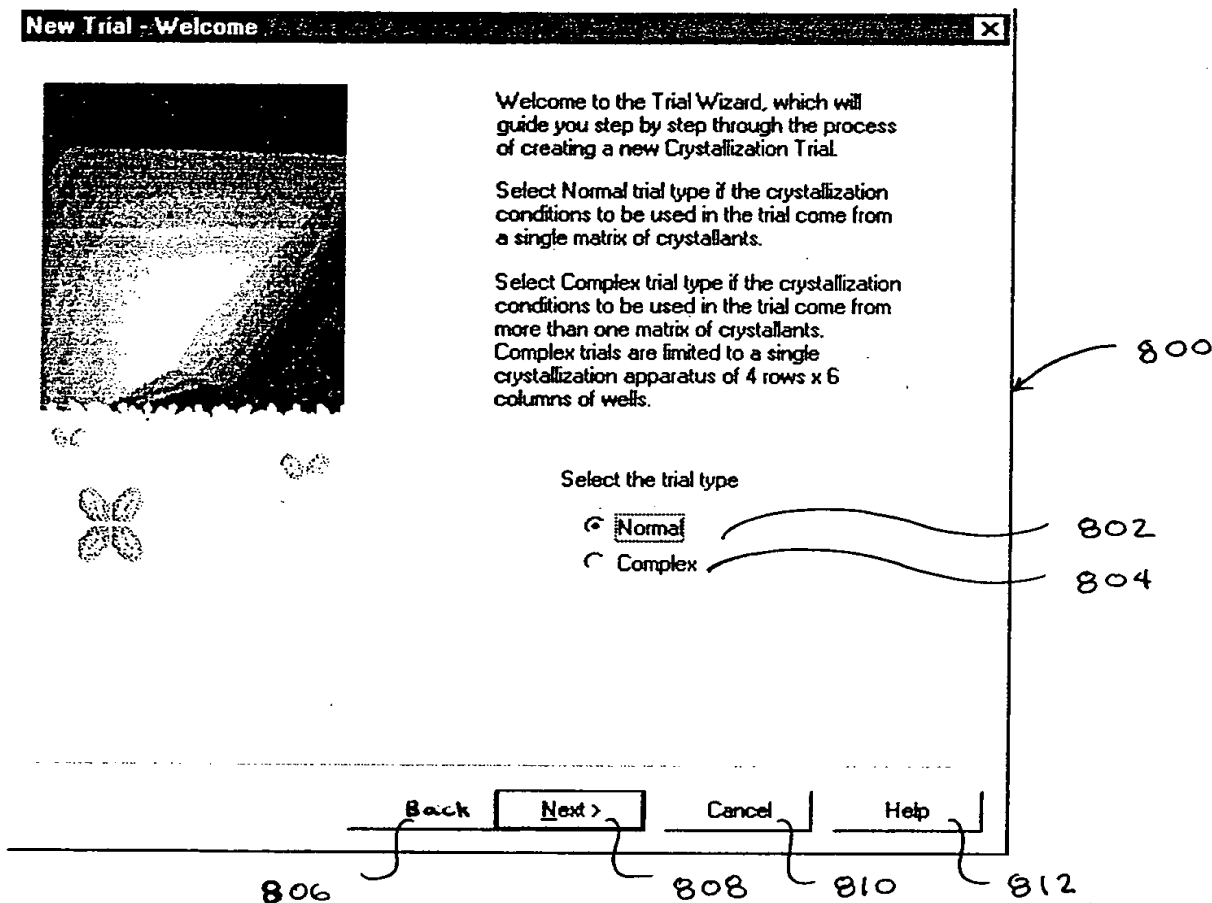


Fig. 8

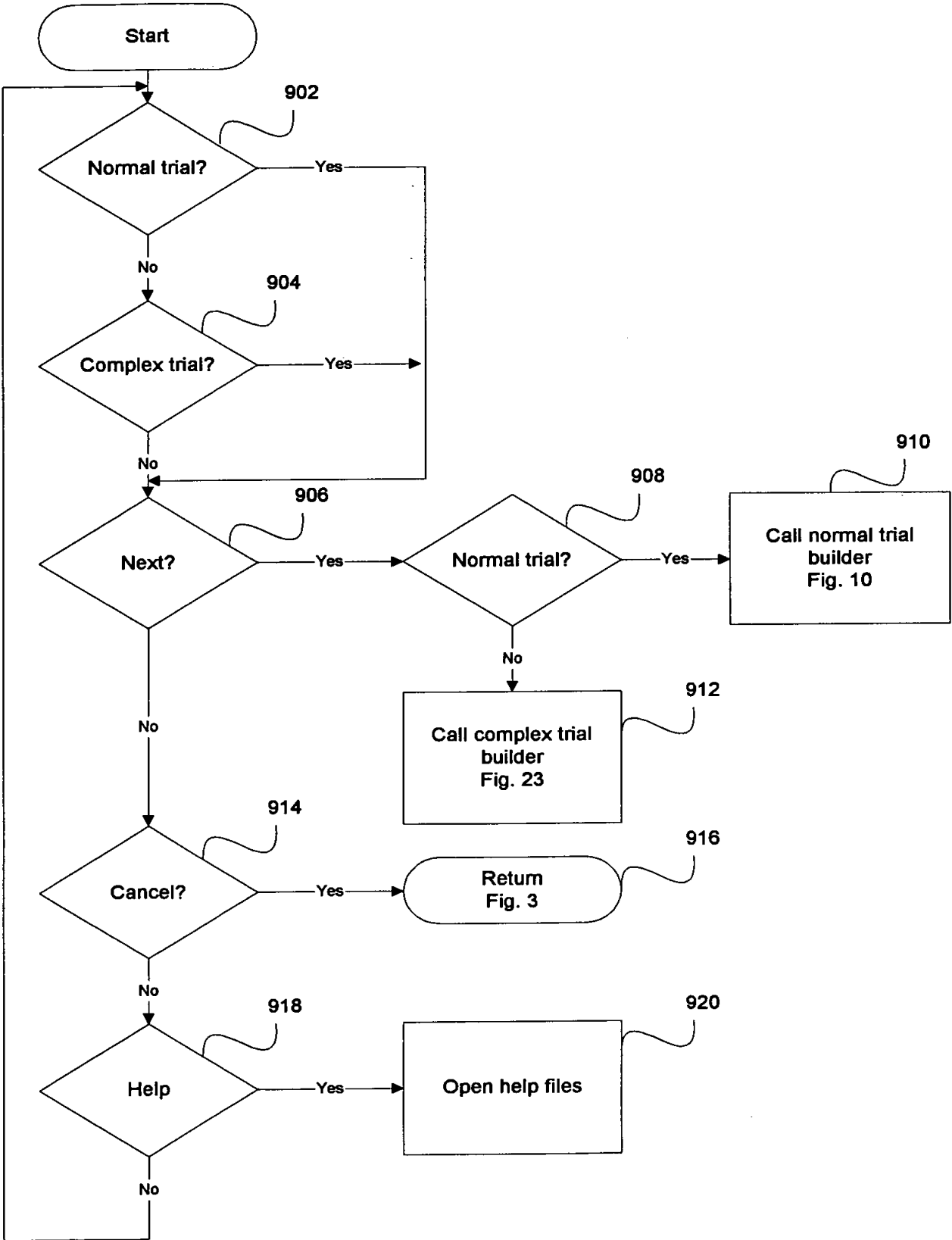


FIGURE 9

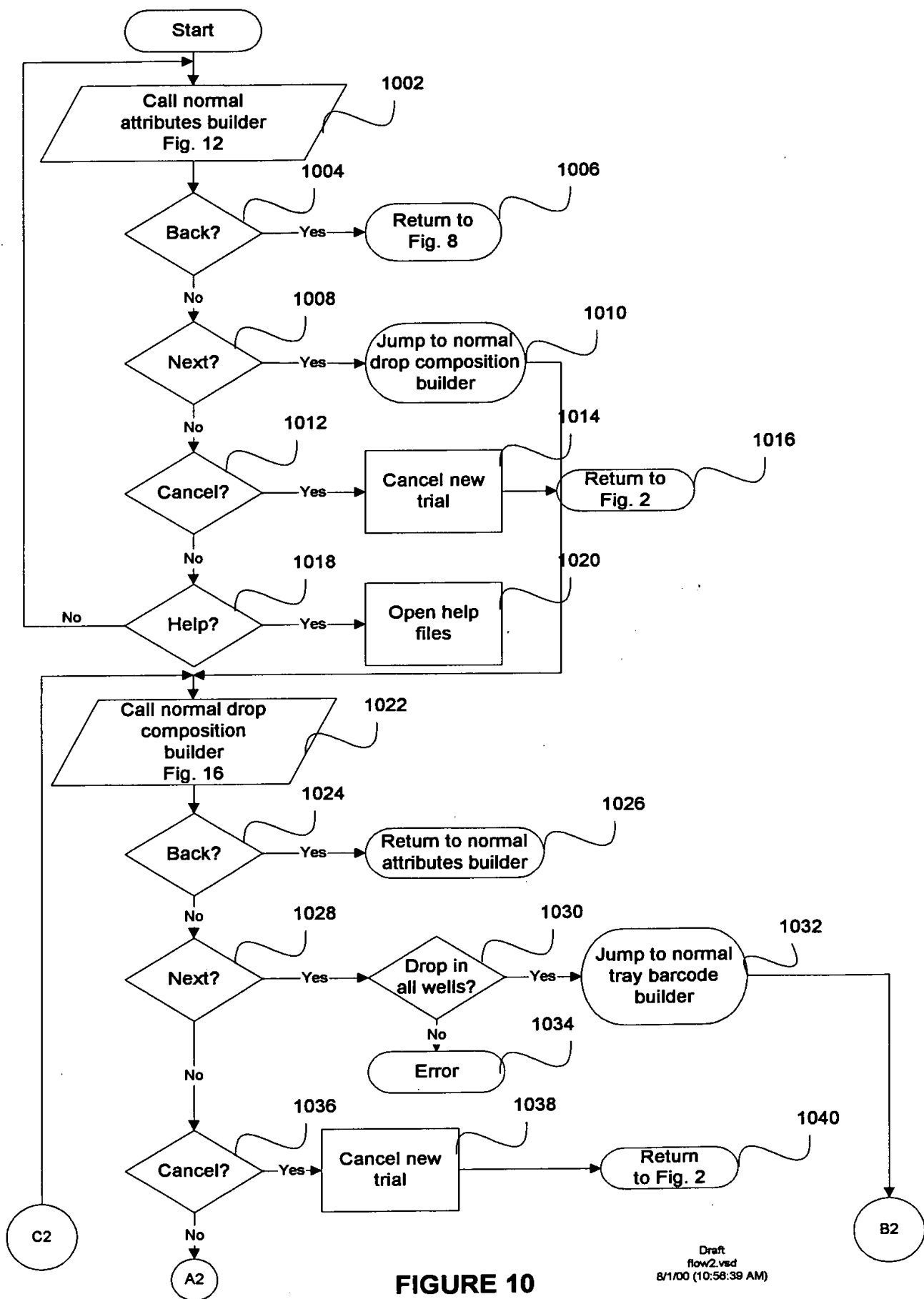


FIGURE 10

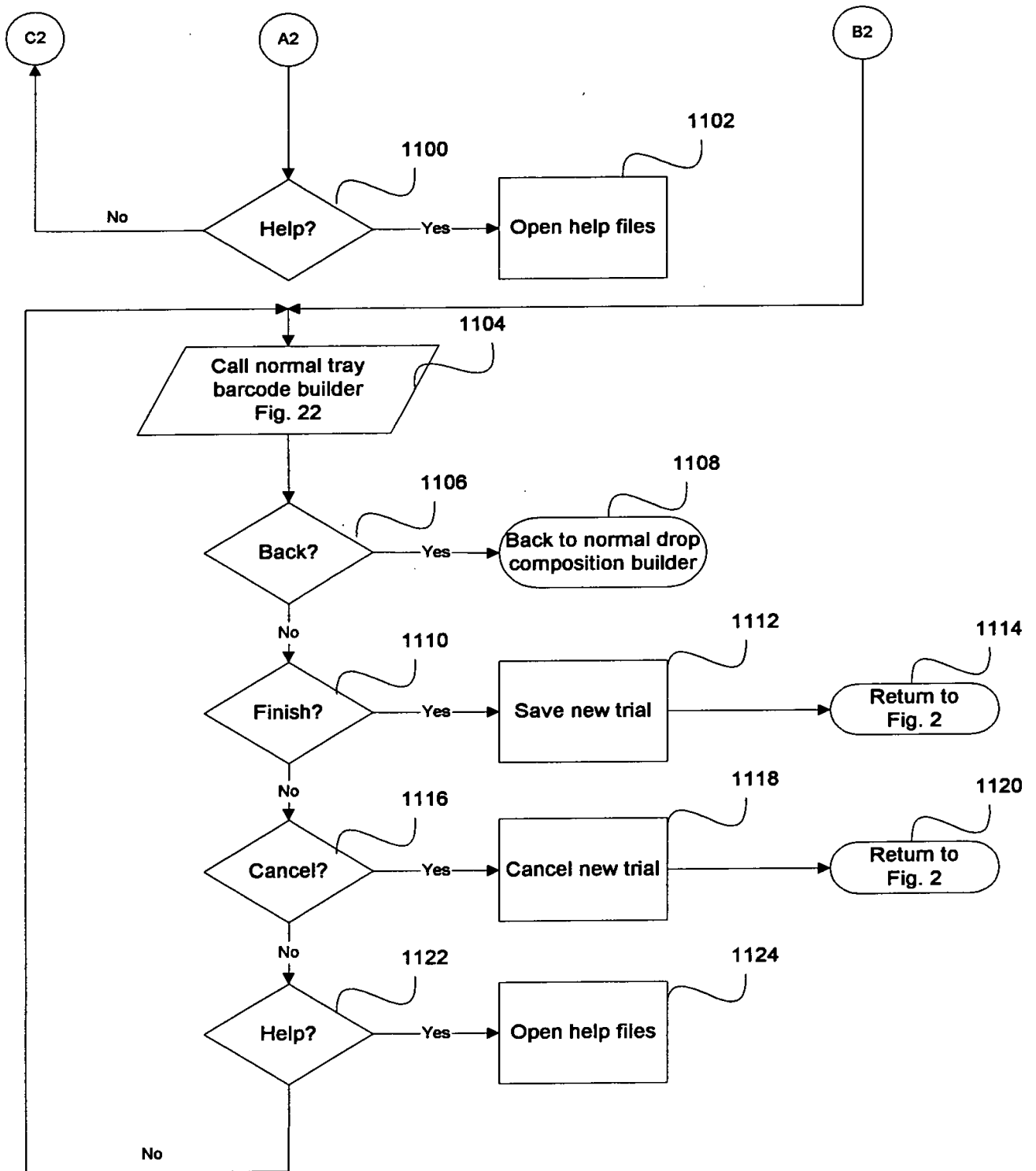
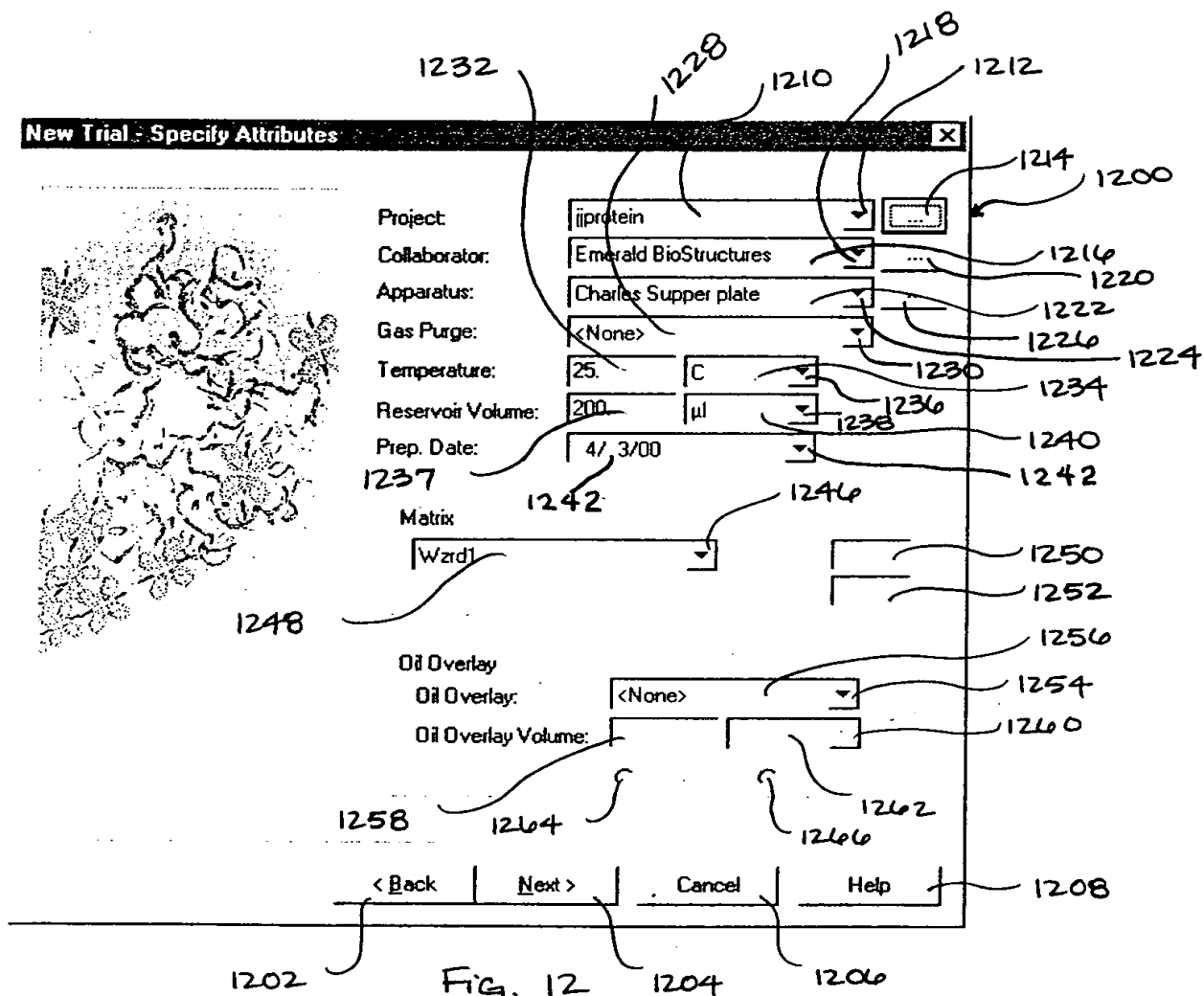


FIGURE 11



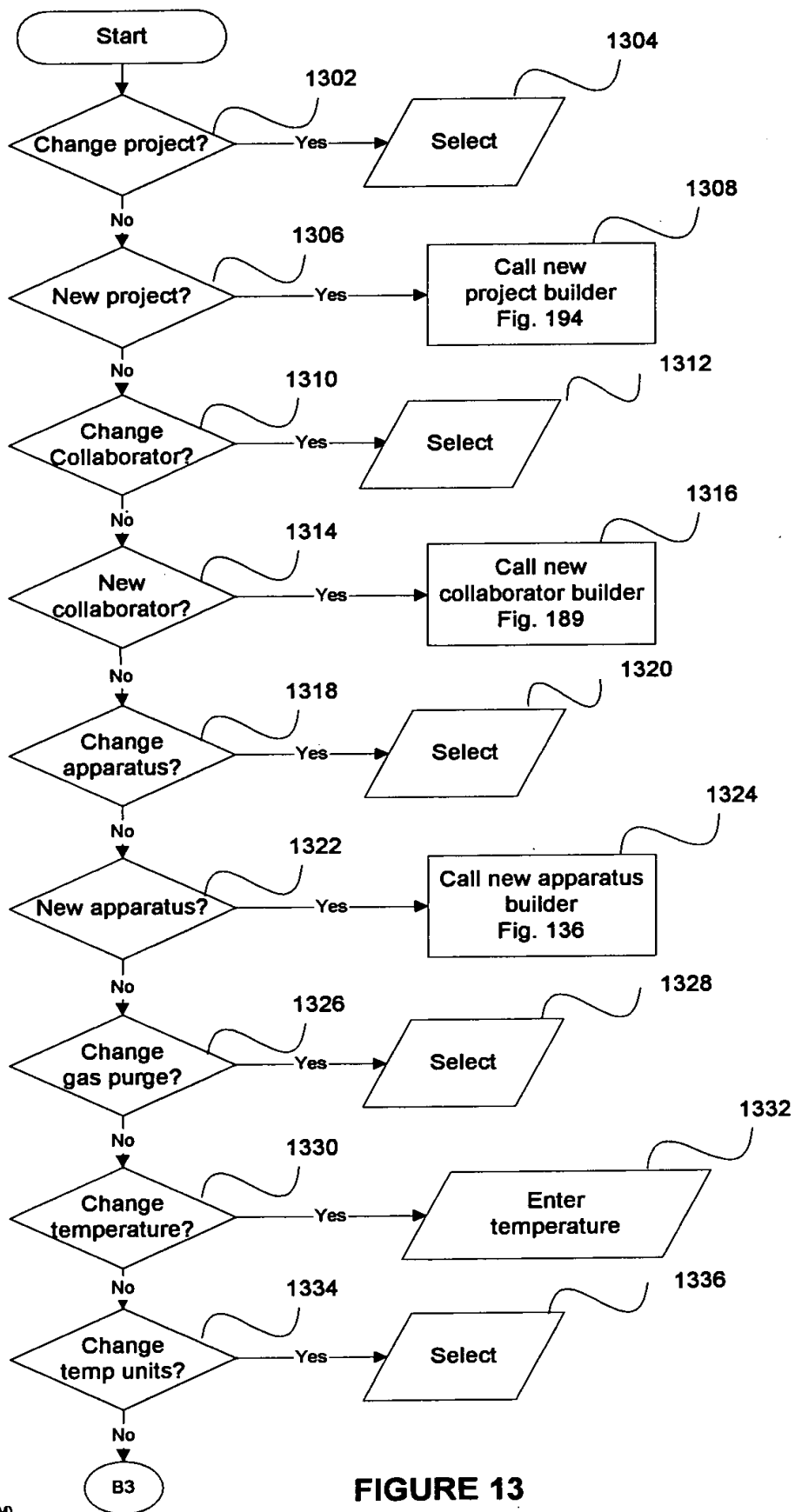


FIGURE 13

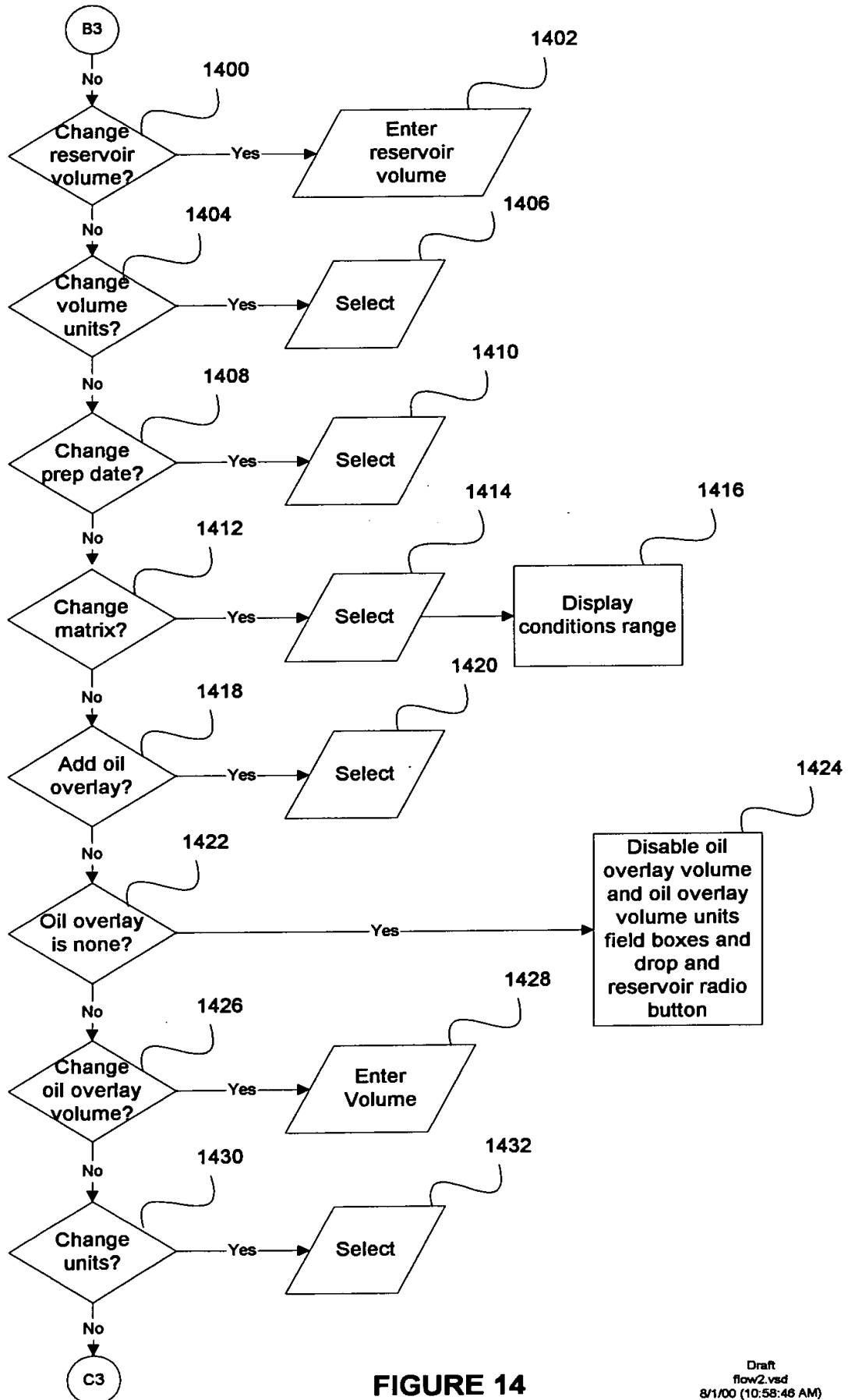
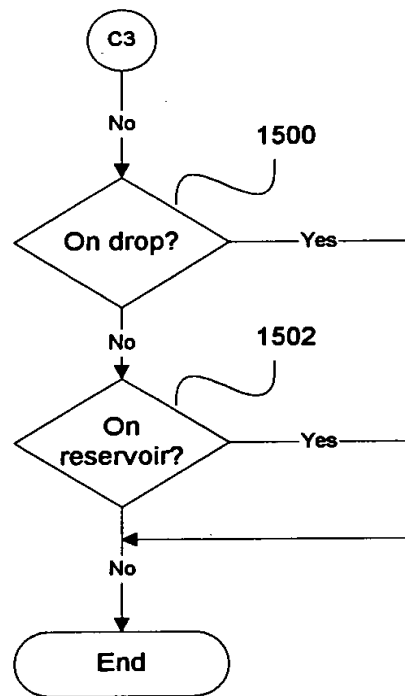


FIGURE 14

002080"58T.E.960



**FIGURE 15**



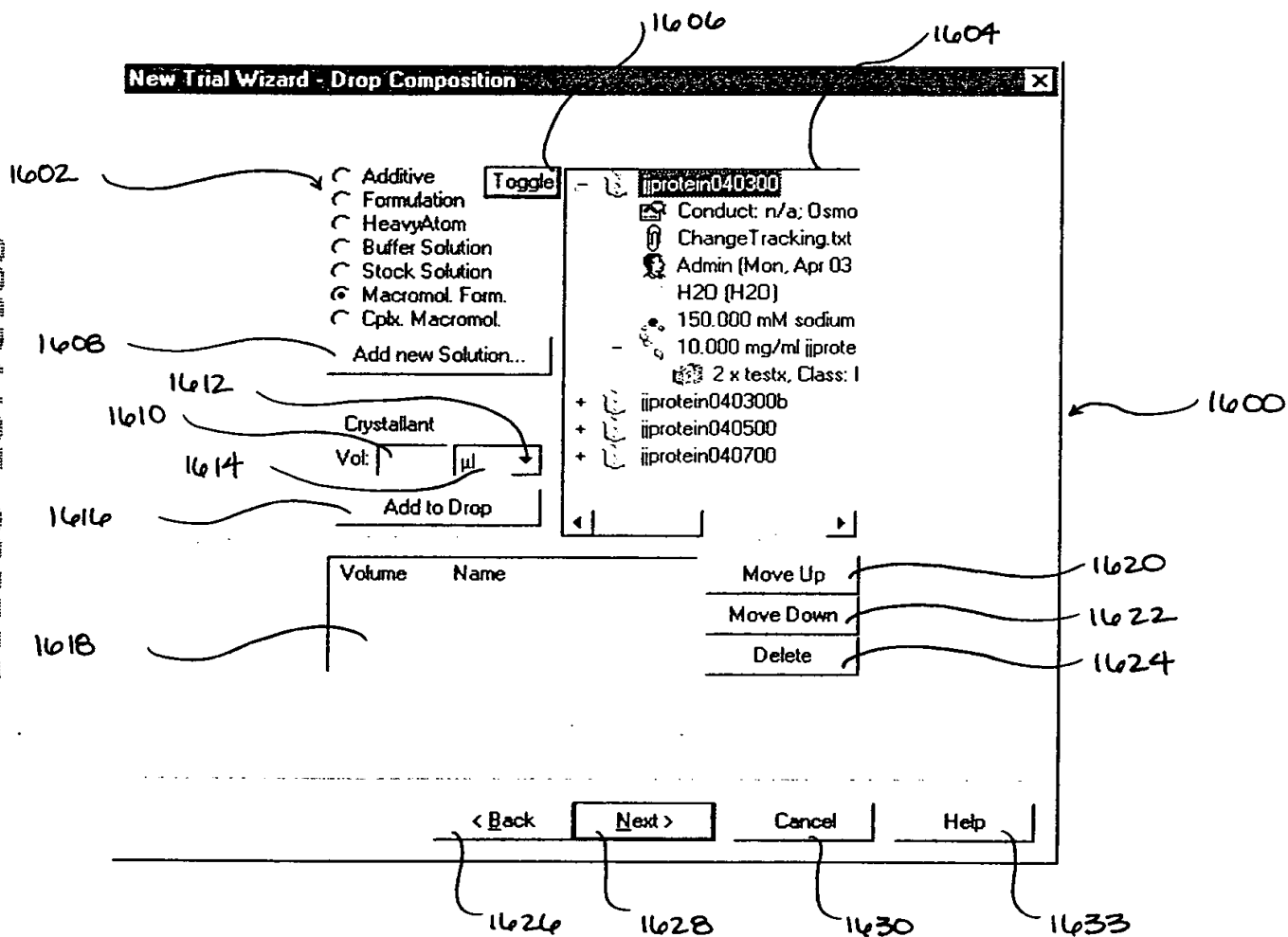


FIG. 116

```

graph TD
    Start([Start]) --> 1700[/Select solution type/]
    1700 --> 1702[Display solution type tree]
    1702 --> 1704{Toggle?}
    1704 -- Yes --> 1706[Toggle between solution list/ solution tree]
    1704 -- No --> 1708{Add a new solution?}
    1708 -- Yes --> 1710[Call new solution builder Fig. 74]
    1708 -- No --> 1712[/Enter crystallant volume/]
    1712 --> 1714{Change Crystallant vol. units?}
    1714 -- Yes --> 1716[/Select/]
    1714 -- No --> 1718{Add crystallant to drop?}
    1718 -- Yes --> 1720[Add to drop list]
    1718 -- No --> 1726([Return])
    1726 --> 1722[/Select solution/]
    1722 --> 1724[Call solution volume builder Fig. 20]
    1724 --> A4((A4))
  
```

**FIGURE 17**

Draft  
flow2.  
8/1/00 (11:0

Draft  
flow2.vsd  
8/1/00 (11:01:52 AM)

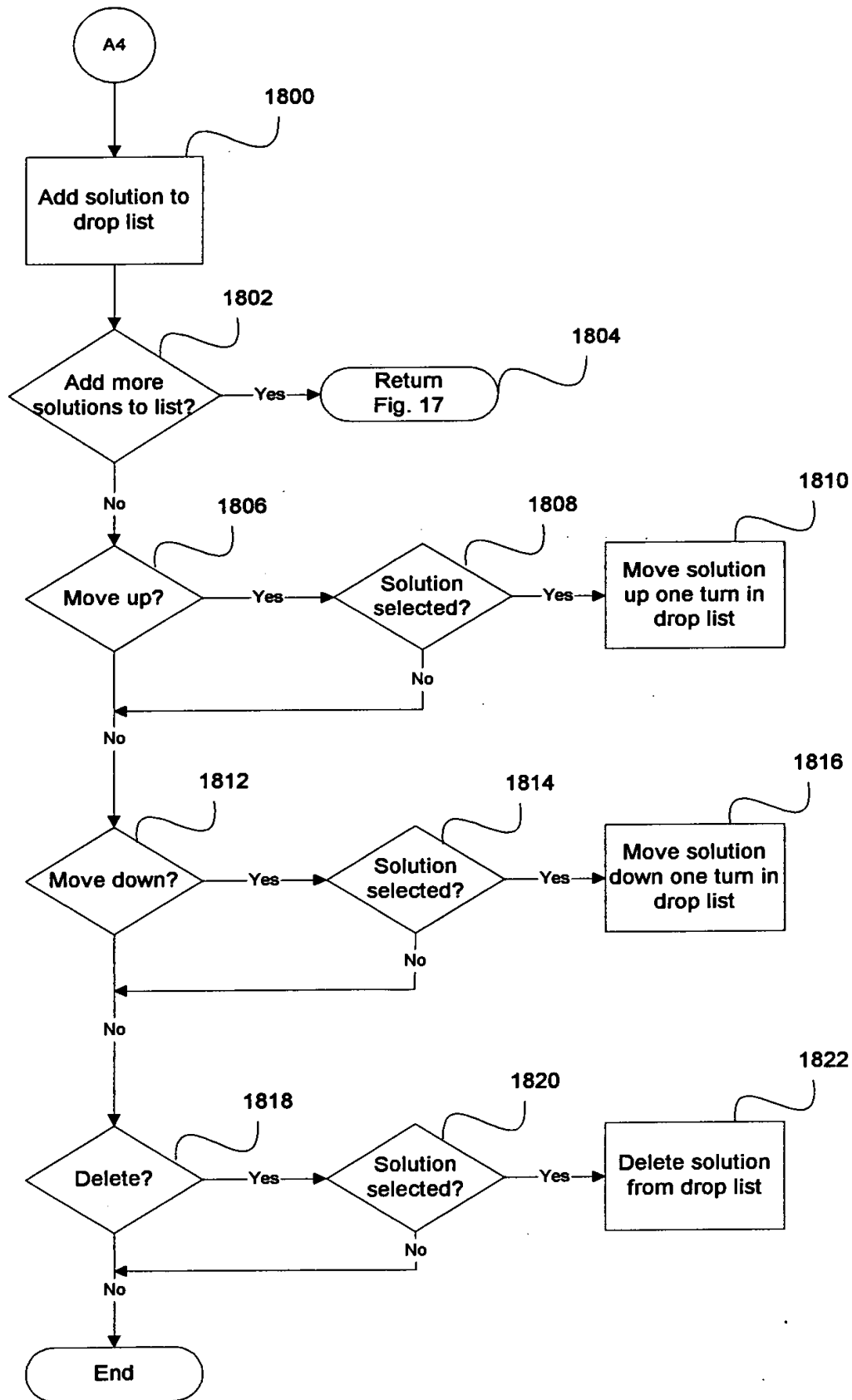


FIGURE 18

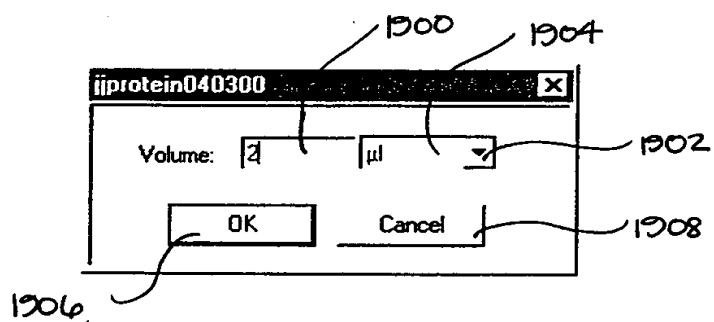


Fig. 19

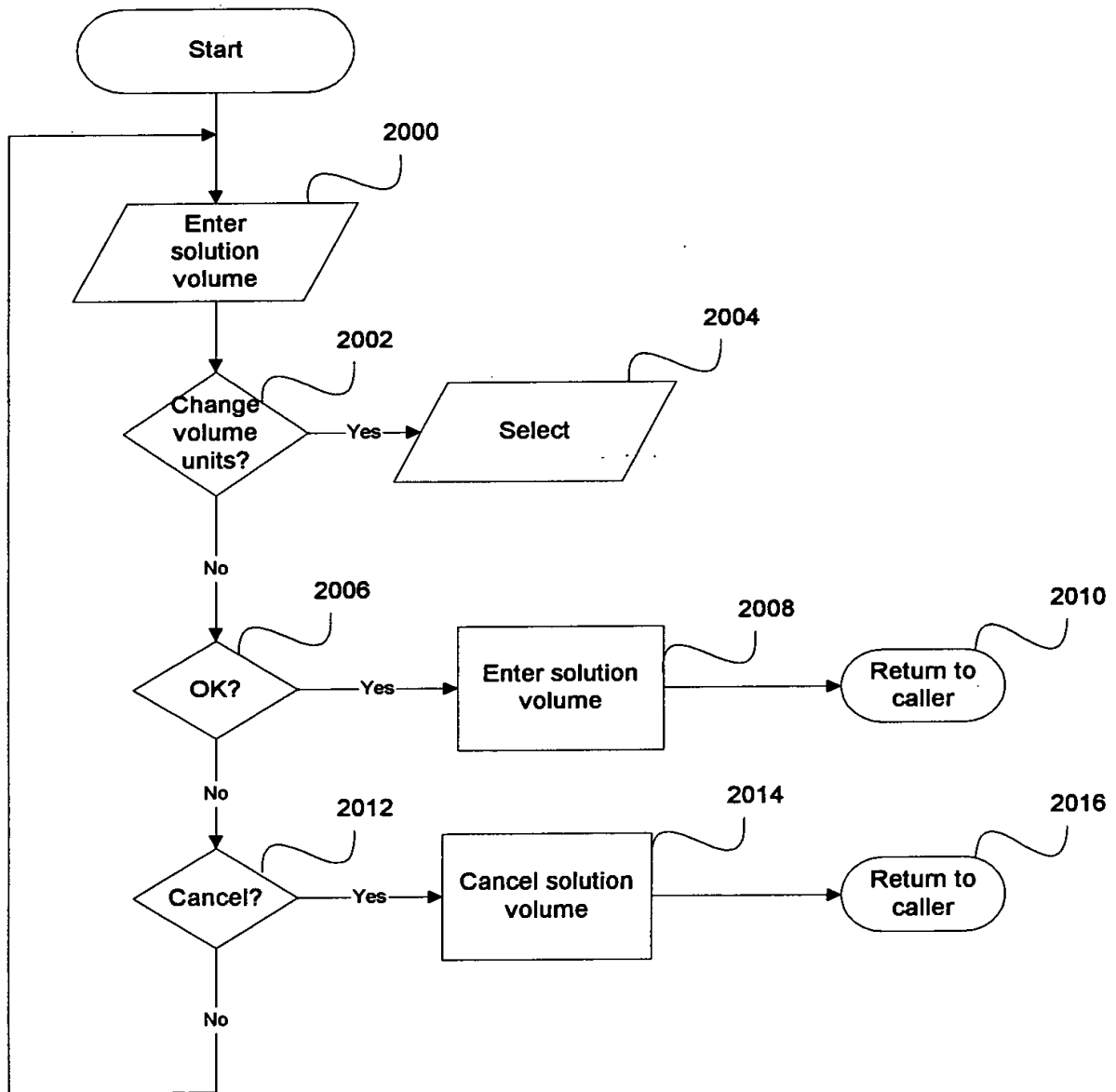


FIGURE 20

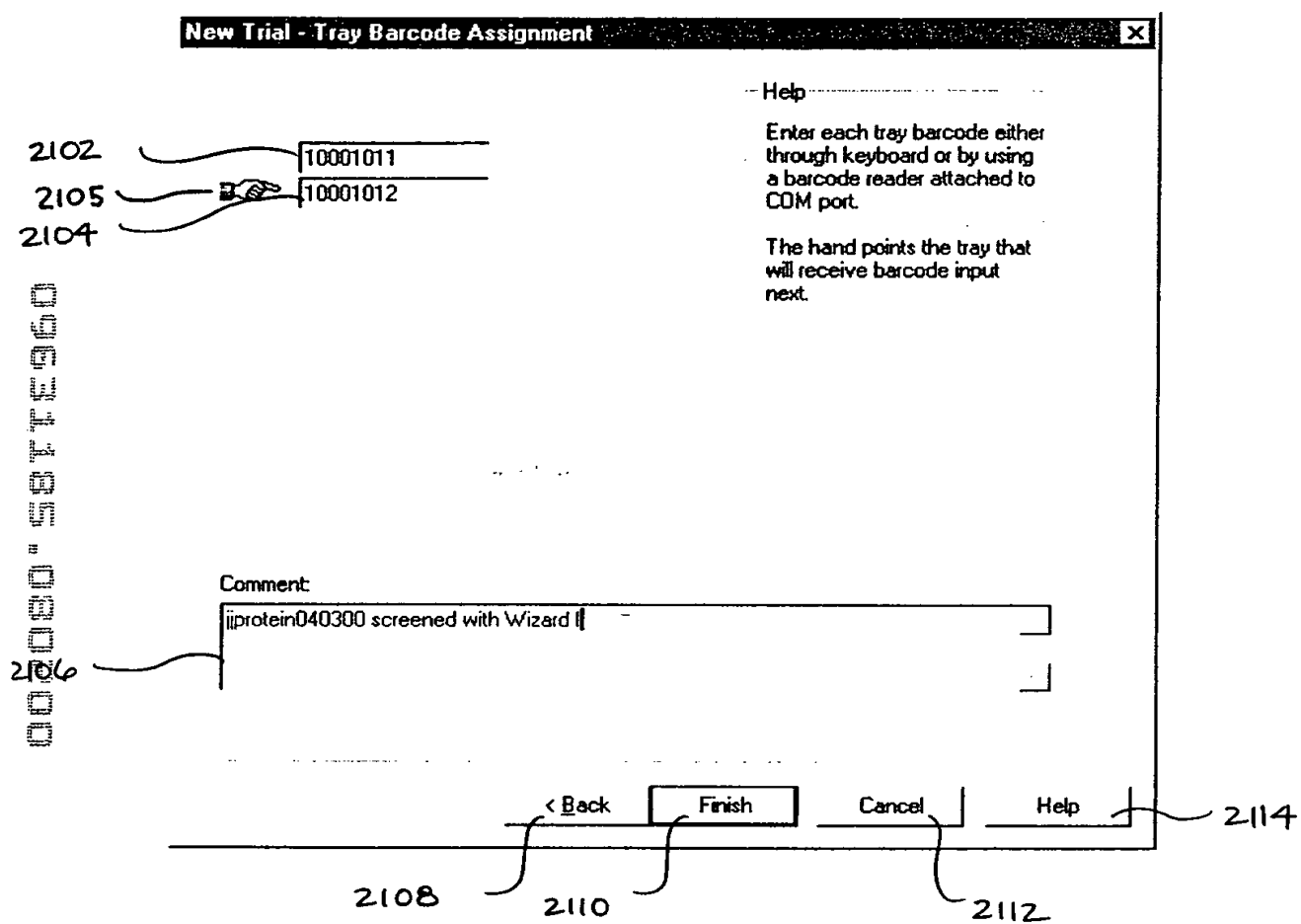
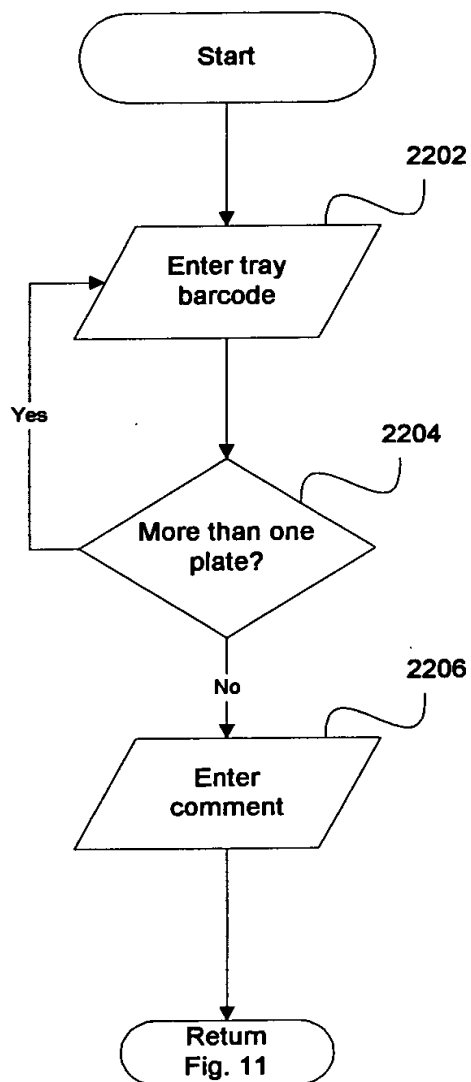


Fig. 21

002080" 5877E950



**FIGURE 22**

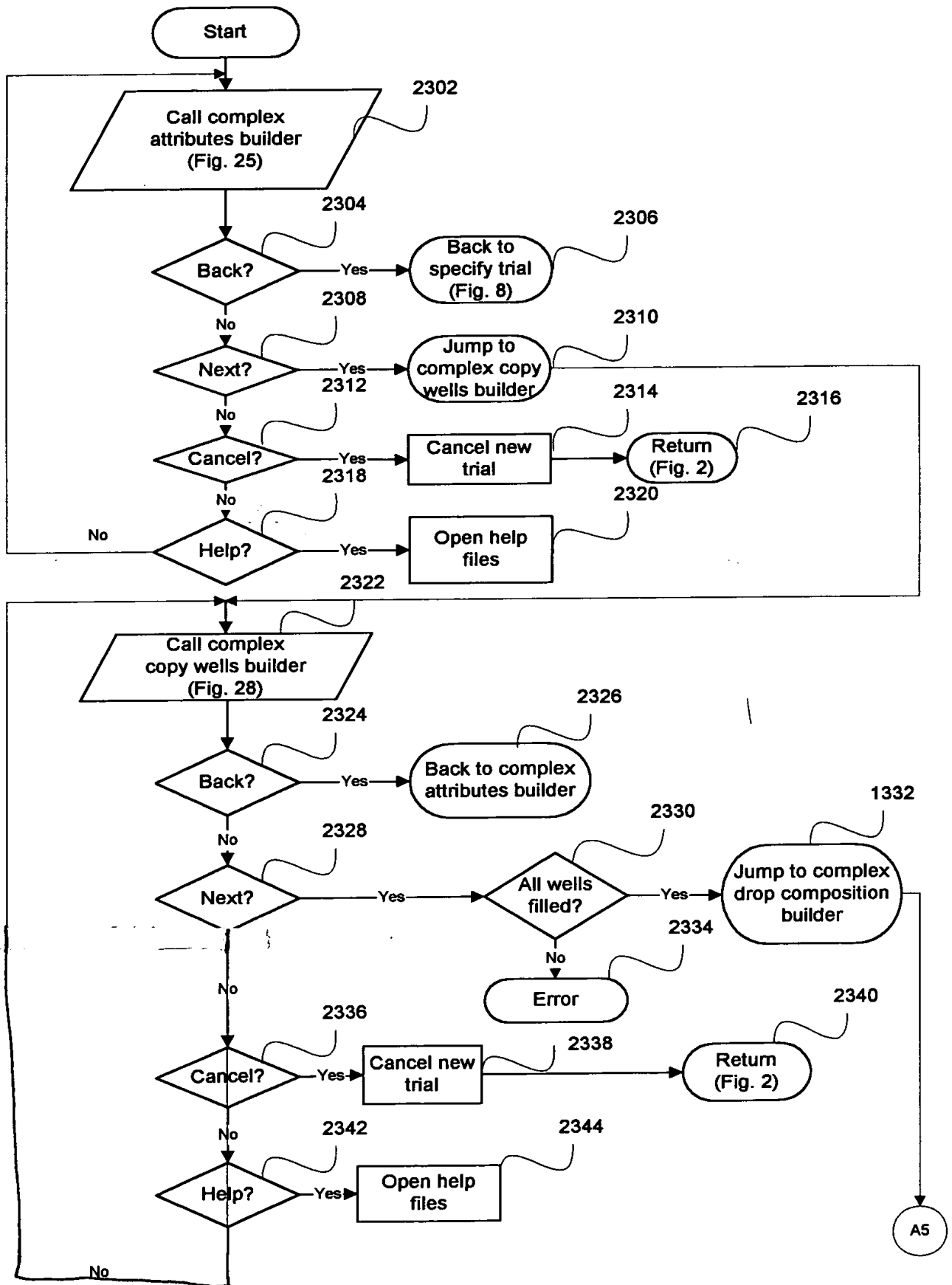
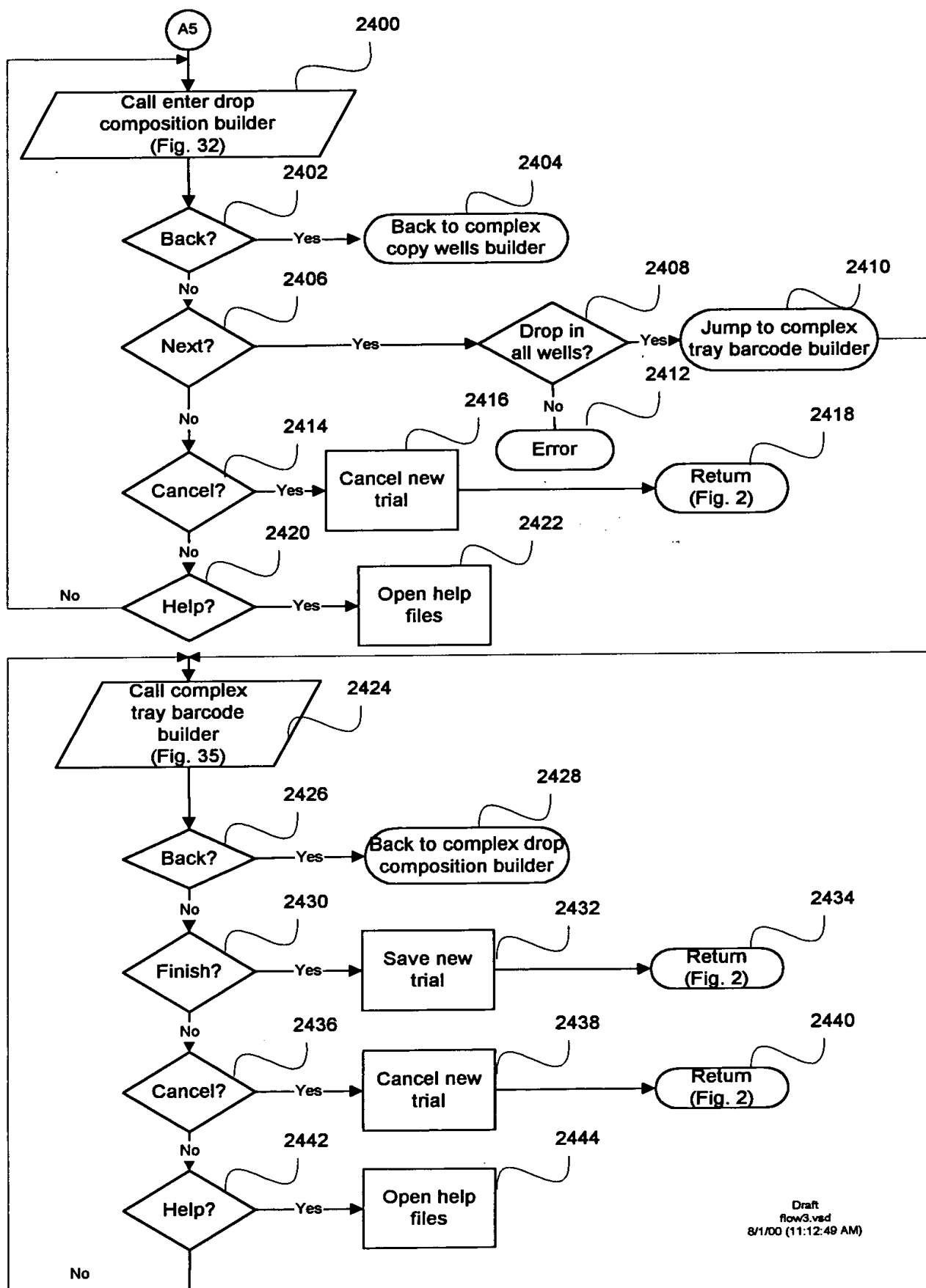


FIGURE 23





Draft  
flow3.vsd  
8/1/00 (11:12:49 AM)

FIGURE 24

**New Trial - Specify Attributes**

Project: protein

Collaborator: Emerald BioStructures

Apparatus: Charles Supper plate

Gas Purge: <None>

Temperature: 25. C

Reservoir Volume: 200. µl

Prep. Date: 4/ 3/00

Oil Overlay

Oil Overlay: <None>

Oil Overlay Volume:

< Back Next > Cancel Help

Callout numbers: 2500, 2528, 2522, 2524, 2514, 2504, 2501, 2502, 2508, 2510, 2506, 2516, 2512, 2518, 2520, 2524, 2530, 2532, 2534, 2536, 2540, 2538, 2542, 2544, 2546, 2550, 2548, 2552, 2554, 2556, 2558.

Fig. 25

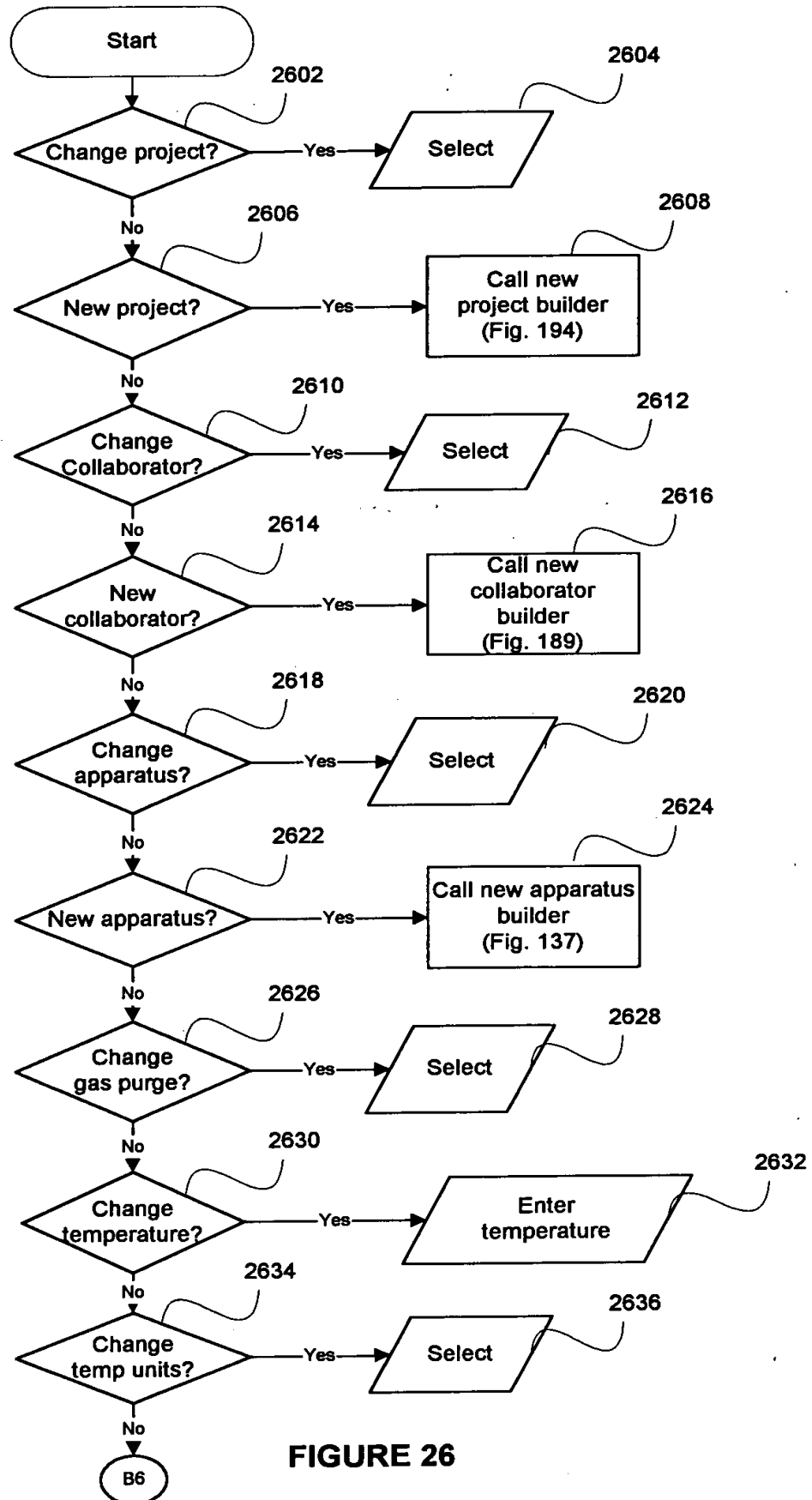


FIGURE 26

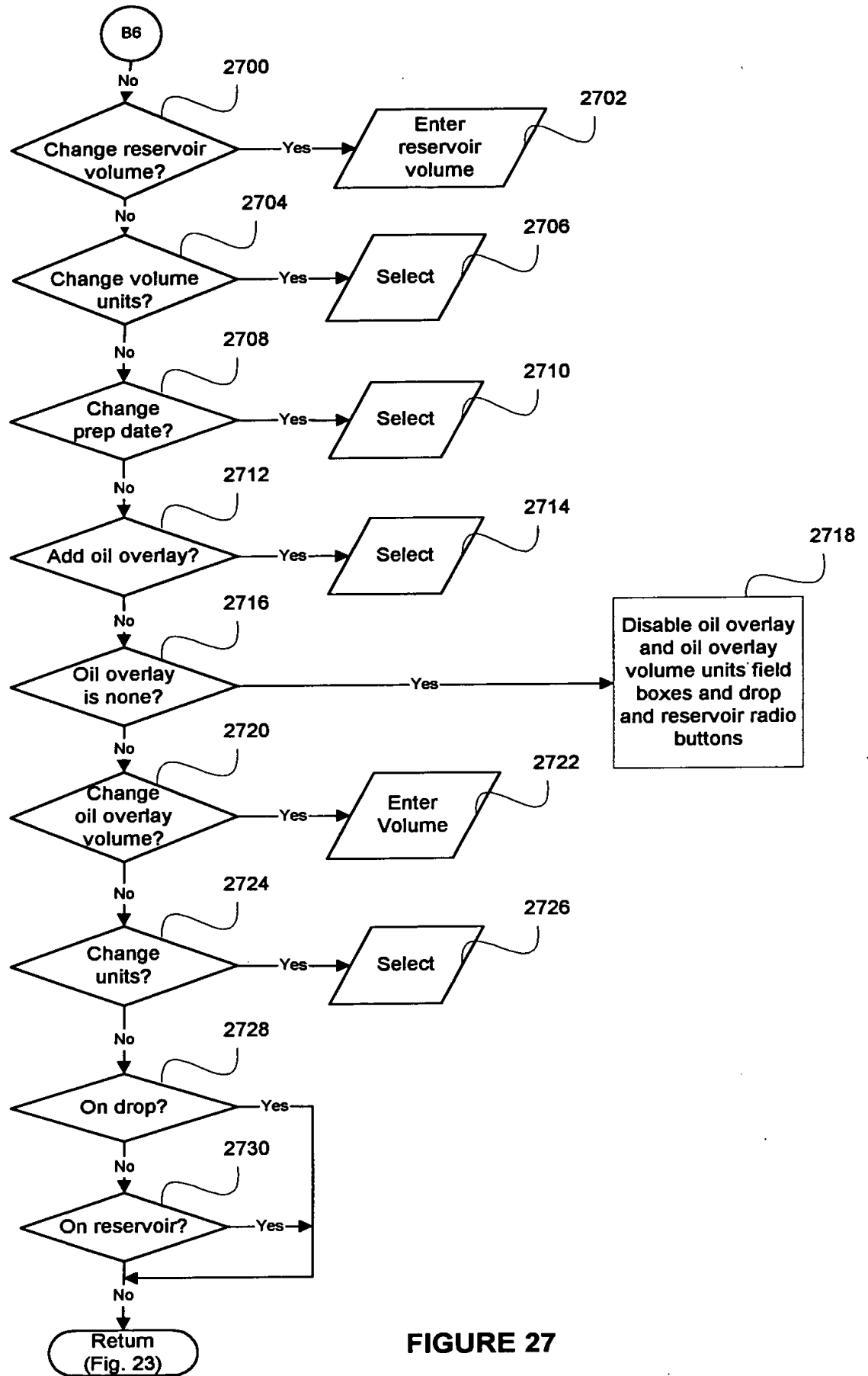


FIGURE 27

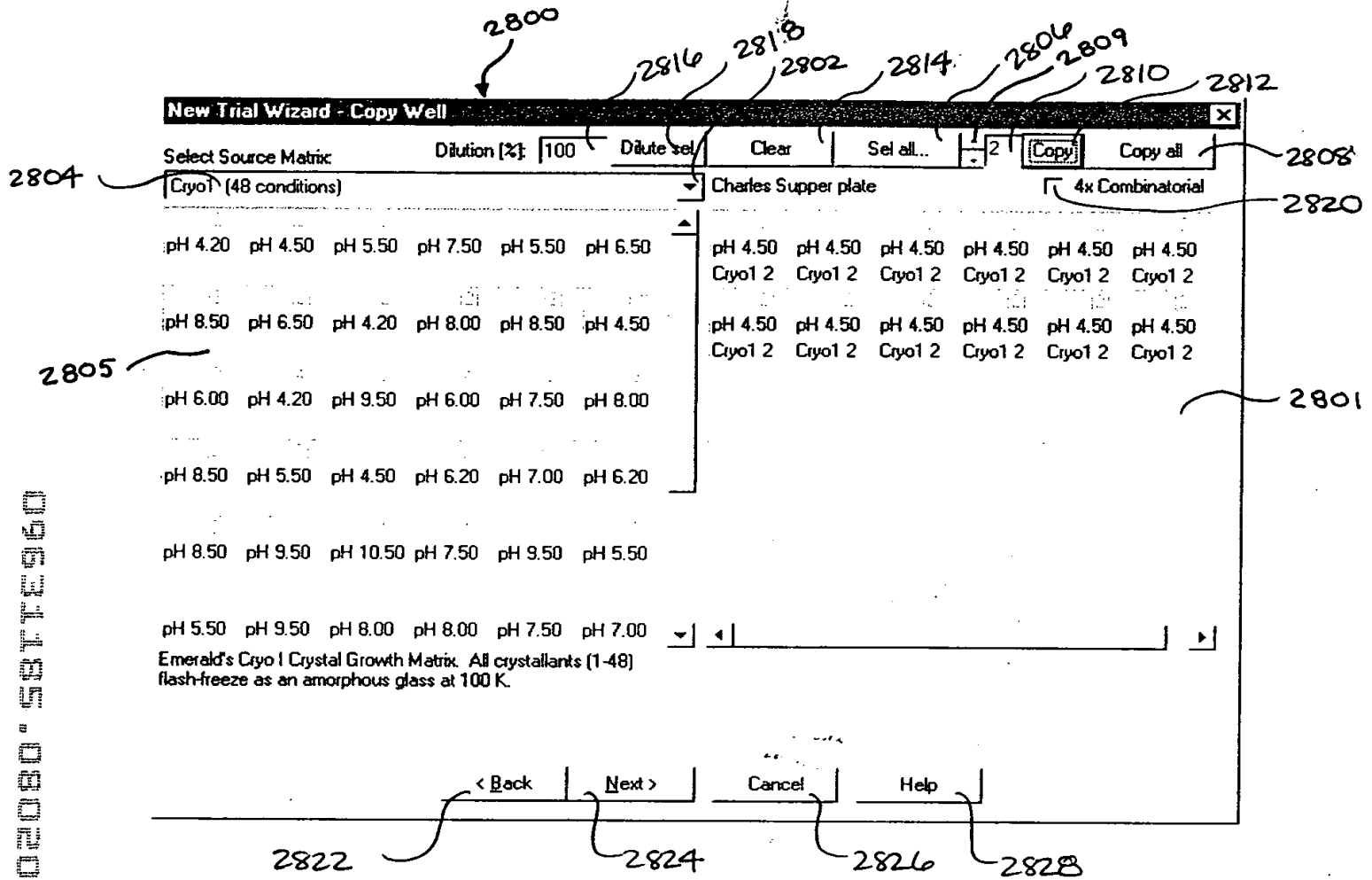


Fig. 28

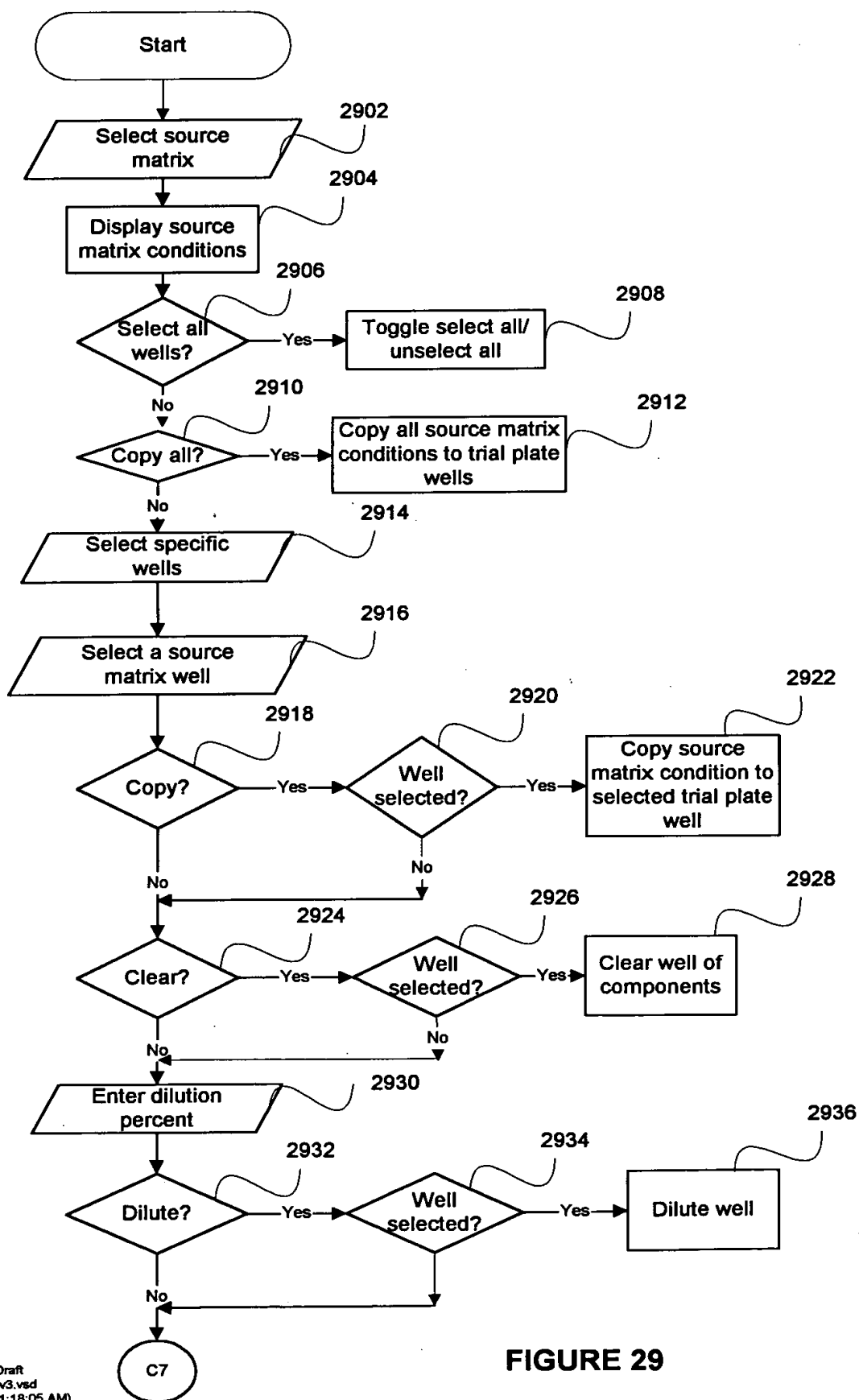
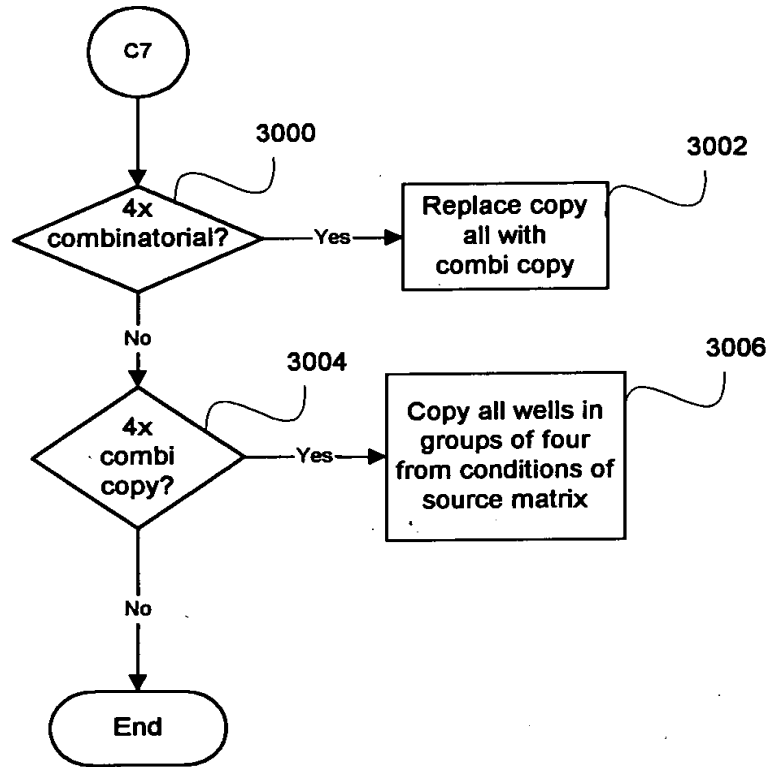


FIGURE 29

002080" 587E560



**FIGURE 30**

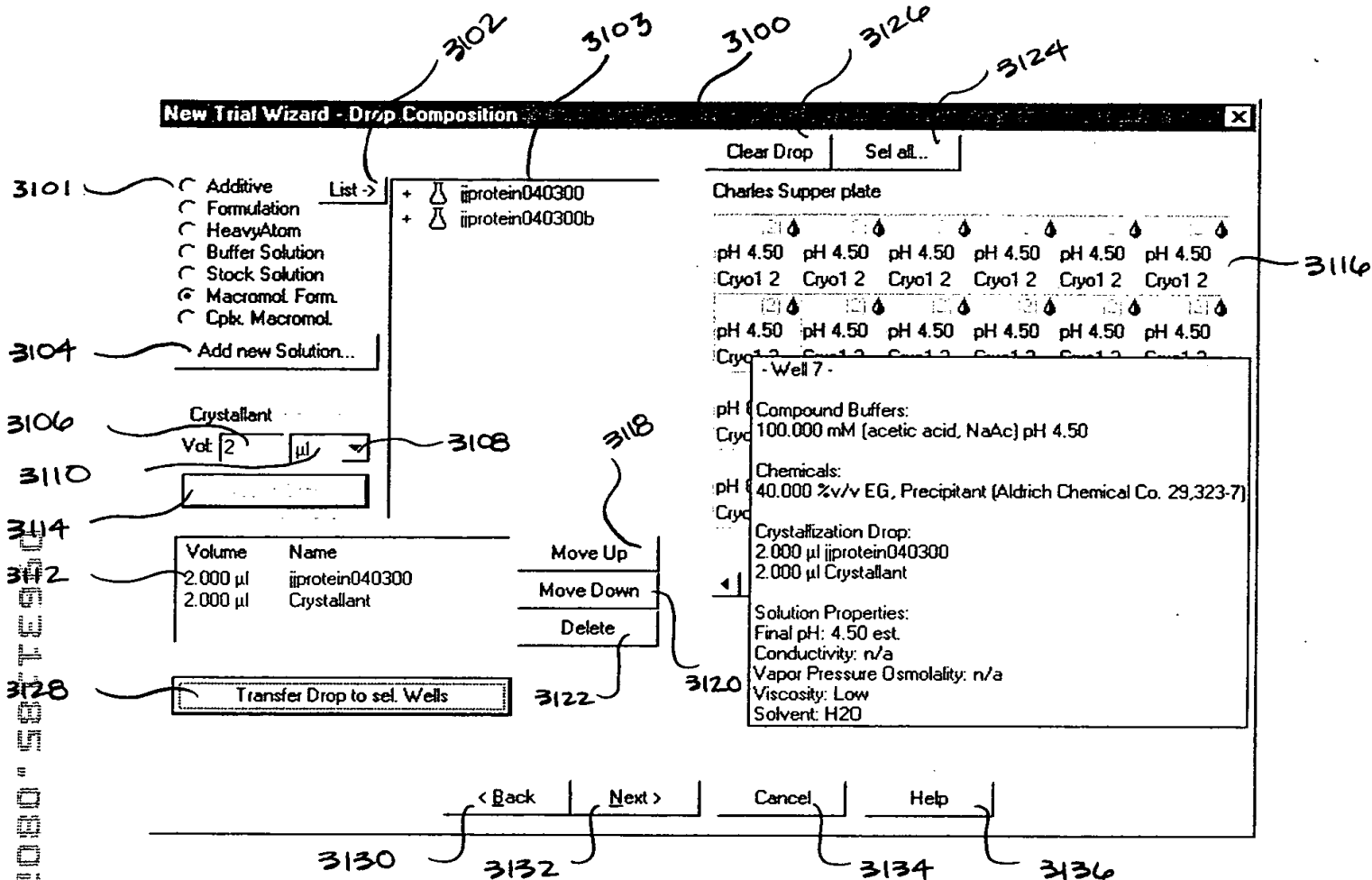


FIG. 31



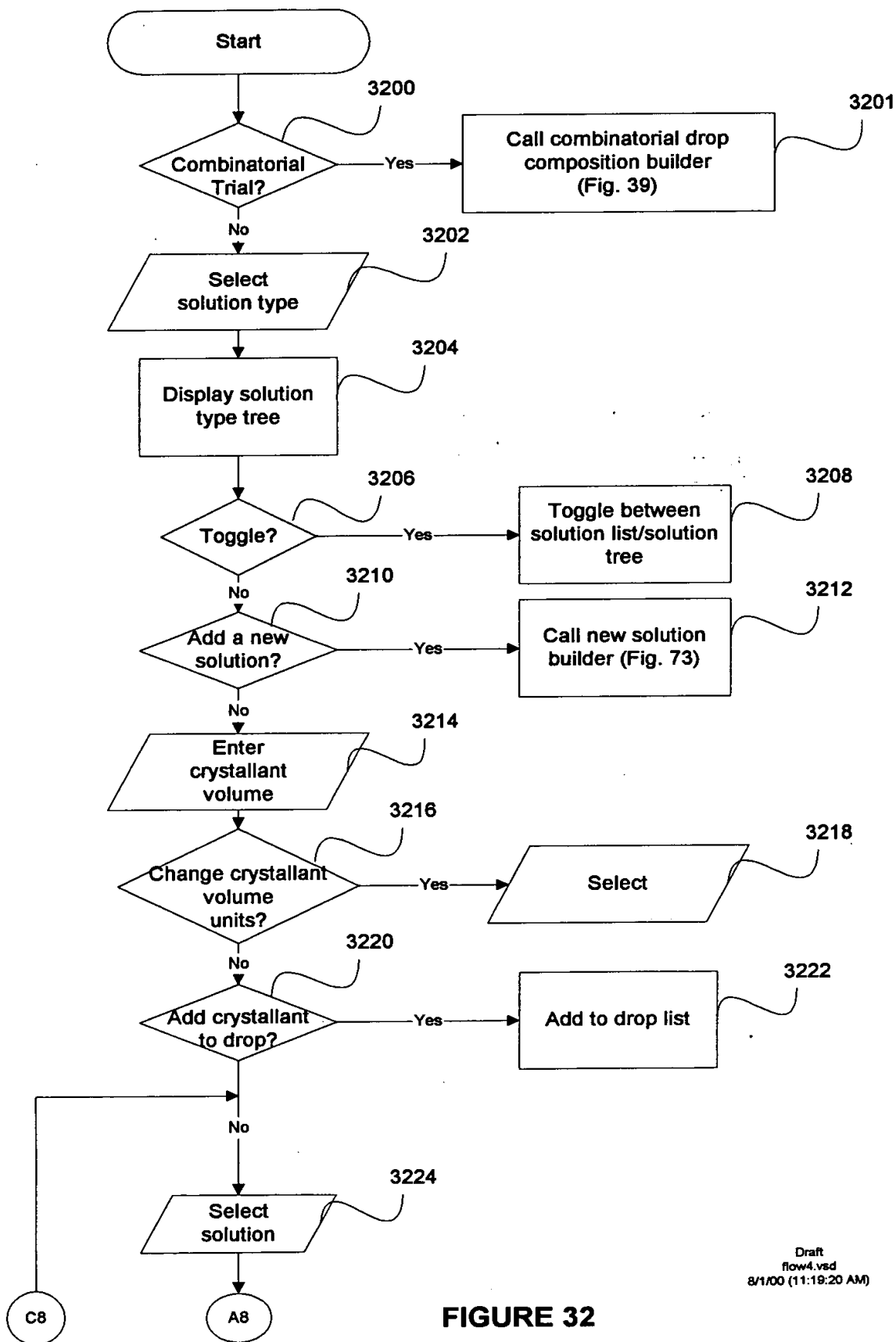


FIGURE 32

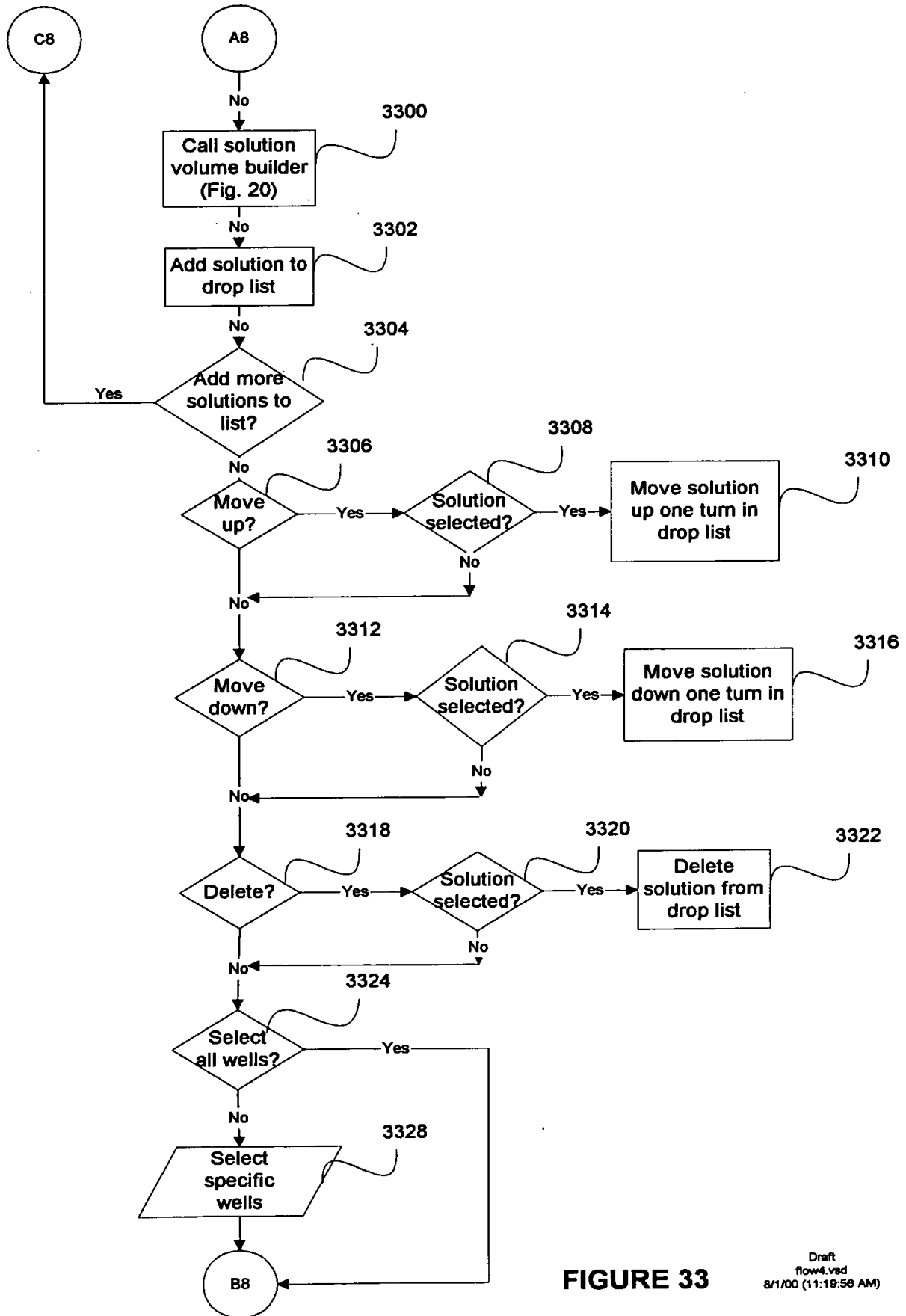


FIGURE 33

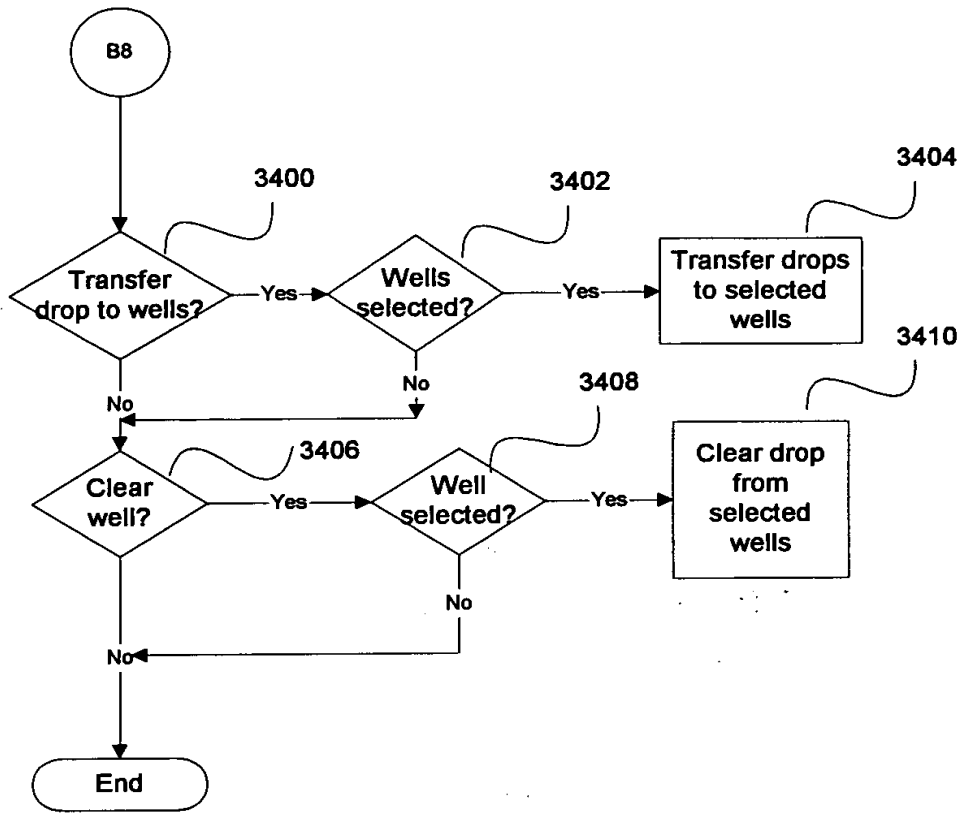


FIGURE 34

002080"587E960

3500

New Trial - Tray Barcode Assignment

3501

10009999

Help

Enter each tray barcode either through keyboard or by using a barcode reader attached to COM port.

The hand points the tray that will receive barcode input next.

Comment

3502

ijprotein040300 in Cryo I #2, and ijprotein040300b in Cryo II #11

3504

< Back

3506

Finish

3508

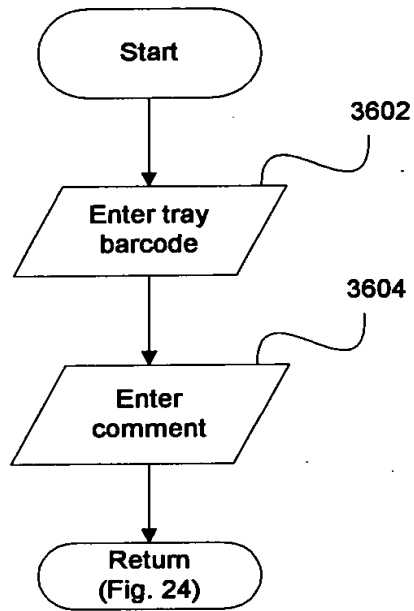
Cancel

Help

3510

Fig. 35

002080" GSTTE960



**FIGURE 36**

3700

3706

New Trial Wizard - Copy Well

Select Source Matrix: Dilution [%]: 100 Dilute sel. Clear Sel all... Copy 4x Combi Copy

3704

Wzrd1 (48 conditions) VDX plate 4x combi ☒ 4x Combinatorial

3708

pH 9.50	pH 7.50	pH 9.50	pH 8.00	pH 10.50	pH 5.50	pH 9.50	pH 9.50	pH 7.50	pH 7.50	pH 9.50	pH 9.50
Wzrd1 1	Wzrd1 1	Wzrd1 2	Wzrd1 2	Wzrd1 3	Wzrd1 1	Wzrd1 1	Wzrd1 1	Wzrd1 2	Wzrd1 2	Wzrd1 3	Wzrd1 1
pH 6.00	pH 5.50	pH 4.50	pH 7.00	pH 6.00	pH 8.00	pH 9.50	pH 9.50	pH 7.50	pH 7.50	pH 9.50	pH 9.50
Wzrd1 1	Wzrd1 1	Wzrd1 2	Wzrd1 2	Wzrd1 3	Wzrd1 1	Wzrd1 1	Wzrd1 1	Wzrd1 2	Wzrd1 2	Wzrd1 3	Wzrd1 1
pH 6.50	pH 6.50	pH 8.00	pH 6.20	pH 4.50	pH 8.00	pH 6.00	pH 6.00	pH 5.50	pH 5.50	pH 4.50	pH 4.50
Wzrd1 7	Wzrd1 7	Wzrd1 8	Wzrd1 8	Wzrd1 9	Wzrd1 1	Wzrd1 7	Wzrd1 7	Wzrd1 8	Wzrd1 8	Wzrd1 9	Wzrd1 1
pH 7.00	pH 8.00	pH 7.50	pH 8.50	pH 8.00	pH 7.00	pH 6.00	pH 6.00	pH 5.50	pH 5.50	pH 4.50	pH 4.50
Wzrd1 7	Wzrd1 7	Wzrd1 8	Wzrd1 8	Wzrd1 9	Wzrd1 1	Wzrd1 7	Wzrd1 7	Wzrd1 8	Wzrd1 8	Wzrd1 9	Wzrd1 1
pH 8.50	pH 9.50	pH 10.50	pH 7.50	pH 9.50	pH 4.50	pH 6.50	pH 6.50	pH 6.50	pH 6.50	pH 8.00	pH 8.00
Wzrd1 13	Wzrd1 13	Wzrd1 14	Wzrd1 14	Wzrd1 15	Wzrd1 1	Wzrd1 13	Wzrd1 13	Wzrd1 14	Wzrd1 14	Wzrd1 15	Wzrd1 1
pH 4.20	pH 6.20	pH 10.50	pH 8.00	pH 4.50	pH 8.00						
Emerald's Wizard 1 Crystal Growth Matrix. A random sparse matrix of crystallants (1-48).											

3702

3701

3710

3712

3714

3716

< Back Next > Cancel Help

FIG. 37

3800

3801

### New Trial Wizard - Drop Composition

☐ Additive  
☐ Formulation  
☐ HeavyAtom  
☐ Buffer Solution  
☐ Stock Solution  
☒ Macromol. Form.  
☐ Cplx. Macromol. Form.

Add new Solution...

Crystallant

Vol:

Add to Drop

Volume	Name
2.00 µl	yyz4810
2.00 µl	Crystallant

Transfer Drop to sel. Wells

Clear Drop Sel all...

CombiClover

(2)	(2)	(3)	(3)	(2)	(2)
pH 9.50	pH 9.50	pH 7.50	pH 7.50	pH 9.50	pH 9.50
Wzrd1 1	Wzrd1 1	Wzrd1 2	Wzrd1 2	Wzrd1 3	Wzrd1 3
(2)	(2)	(3)	(3)	(2)	(2)
pH 9.50	pH 9.50	pH 7.50	pH 7.50	pH 9.50	pH 9.50
Wzrd1 1	Wzrd1 1	Wzrd1 2	Wzrd1 2	Wzrd1 3	Wzrd1 3
(3)	(3)	(2)	(2)	(2)	(2)
pH 6.00	pH 6.00	pH 5.50	pH 5.50	pH 4.50	pH 4.50
Wzrd1 7	Wzrd1 7	Wzrd1 8	Wzrd1 8	Wzrd1 9	Wzrd1 9
(3)	(3)	(2)	(2)	(2)	(2)
pH 6.00	pH 6.00	pH 5.50	pH 5.50	pH 4.50	pH 4.50
Wzrd1 7	Wzrd1 7	Wzrd1 8	Wzrd1 8	Wzrd1 9	Wzrd1 9
(2)	(2)	(2)	(2)	(3)	(3)
pH 6.50	pH 6.50	pH 6.50	pH 6.50	pH 8.00	pH 8.00
Wzrd1 13	Wzrd1 13	Wzrd1 14	Wzrd1 14	Wzrd1 15	Wzrd1 15
(2)	(2)	(2)	(2)	(2)	(2)
pH 6.50	pH 6.50	pH 6.50	pH 6.50	pH 8.00	pH 8.00
Wzrd1 13	Wzrd1 13	Wzrd1 14	Wzrd1 14	Wzrd1 15	Wzrd1 15

< Back
Next >
Cancel
Help

3802

3804

3806

3808

3810

Fig. 38

002090" 587E960

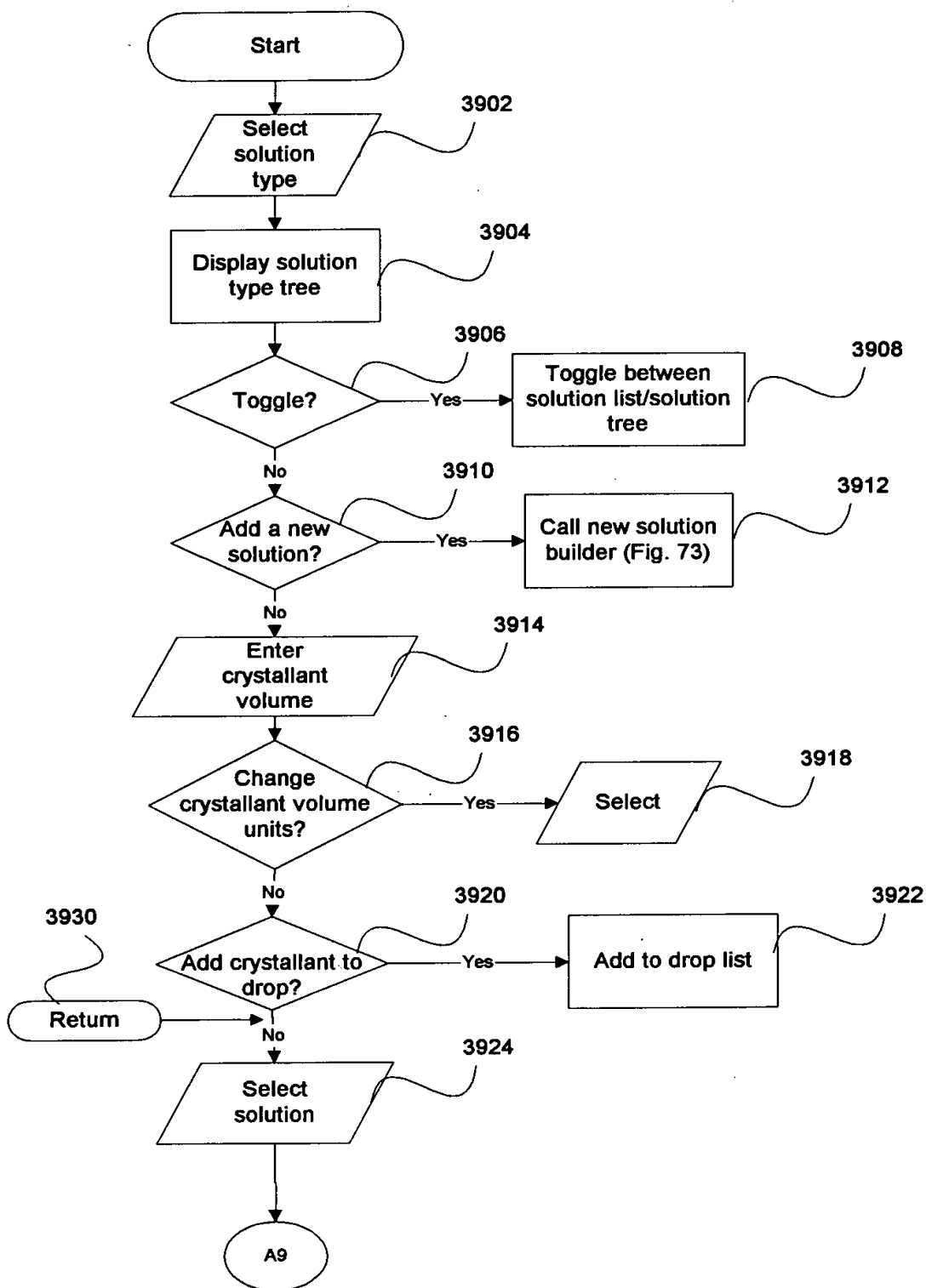


FIGURE 39



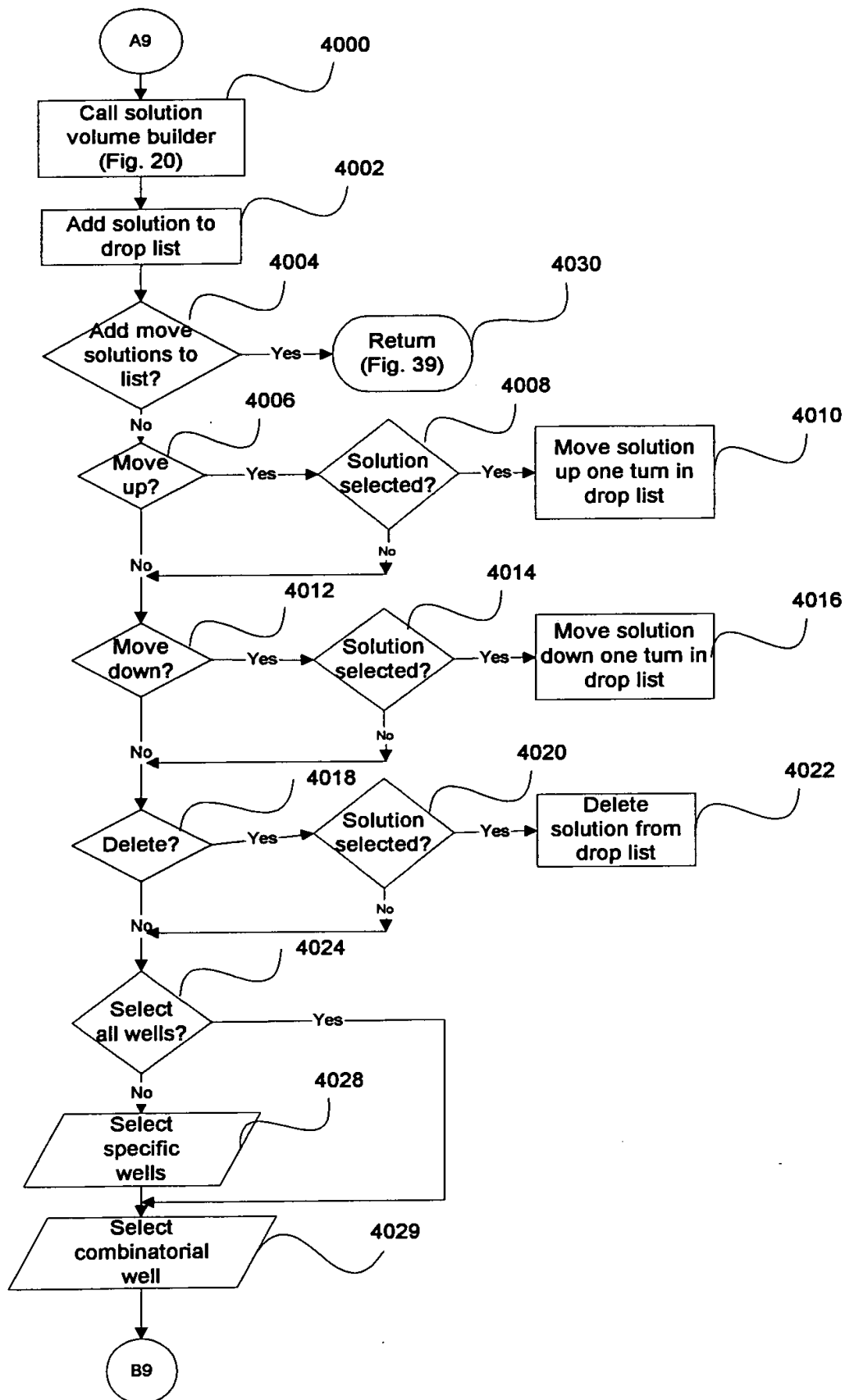


FIGURE 40

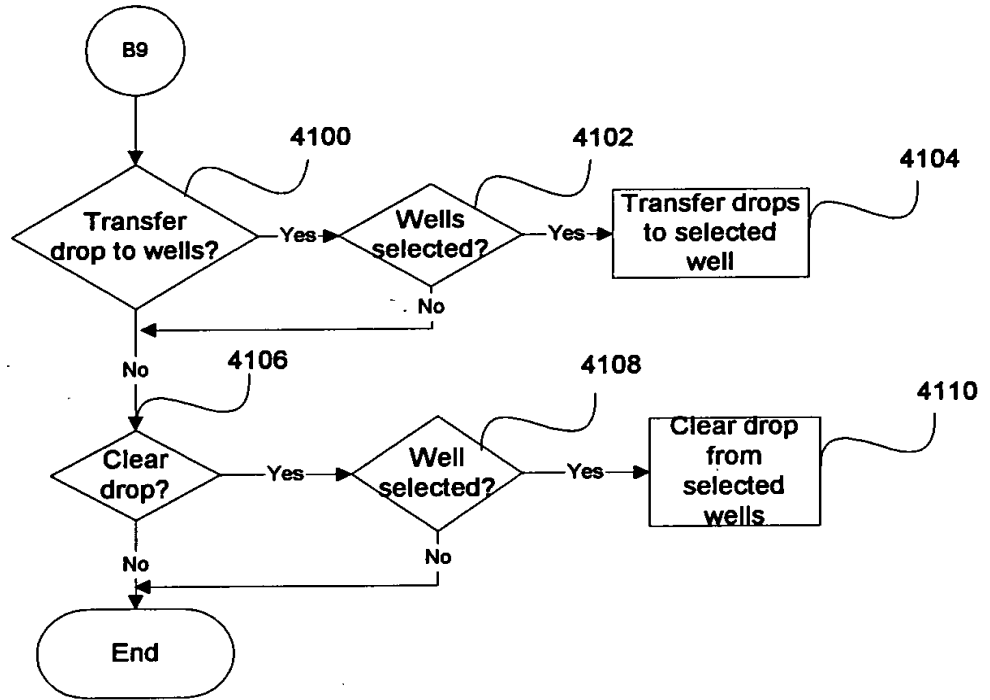
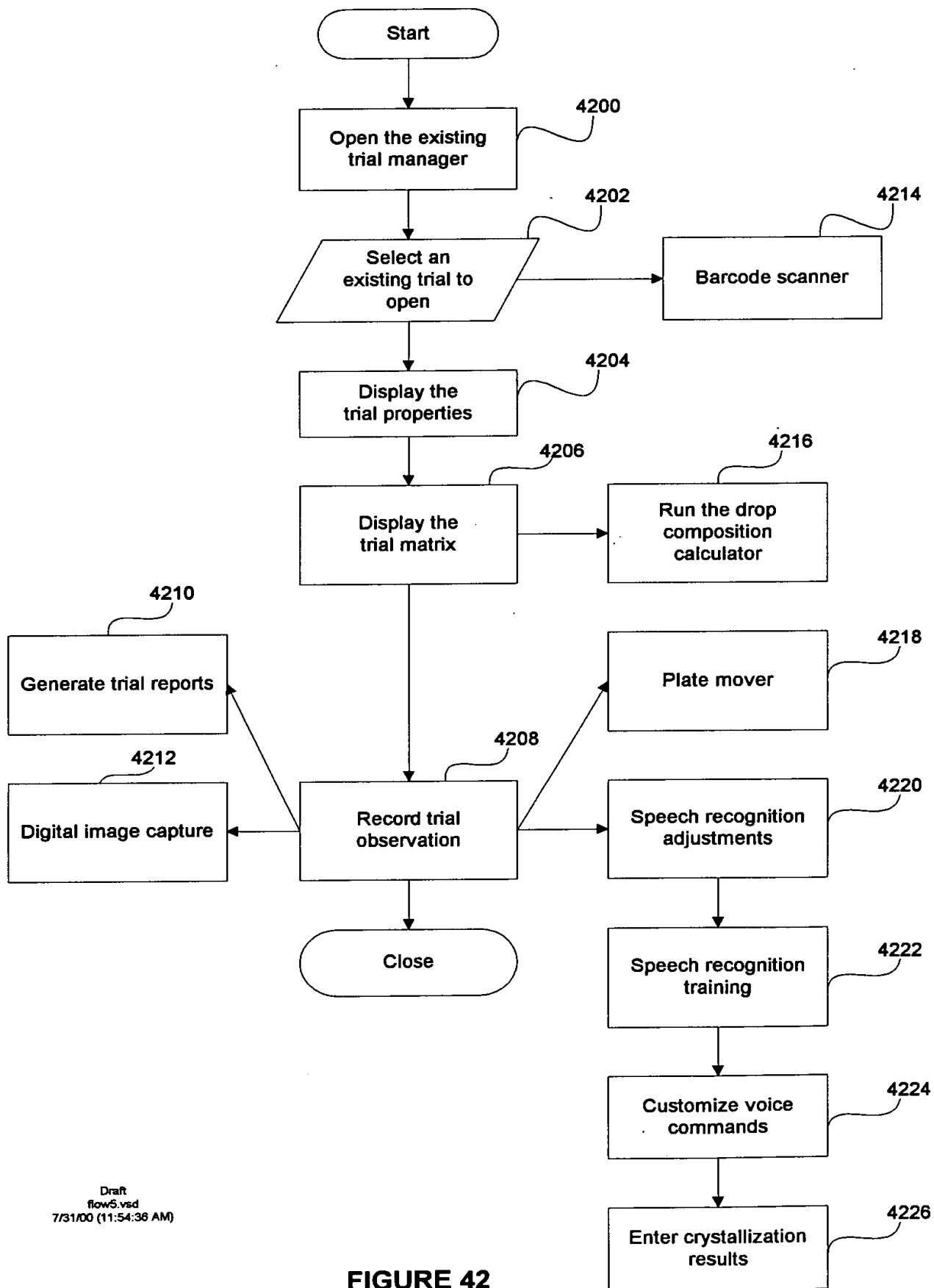


FIGURE 41



Draft  
flow5.vsd  
7/31/00 (11:54:36 AM)

FIGURE 42

002080" 58TTE960

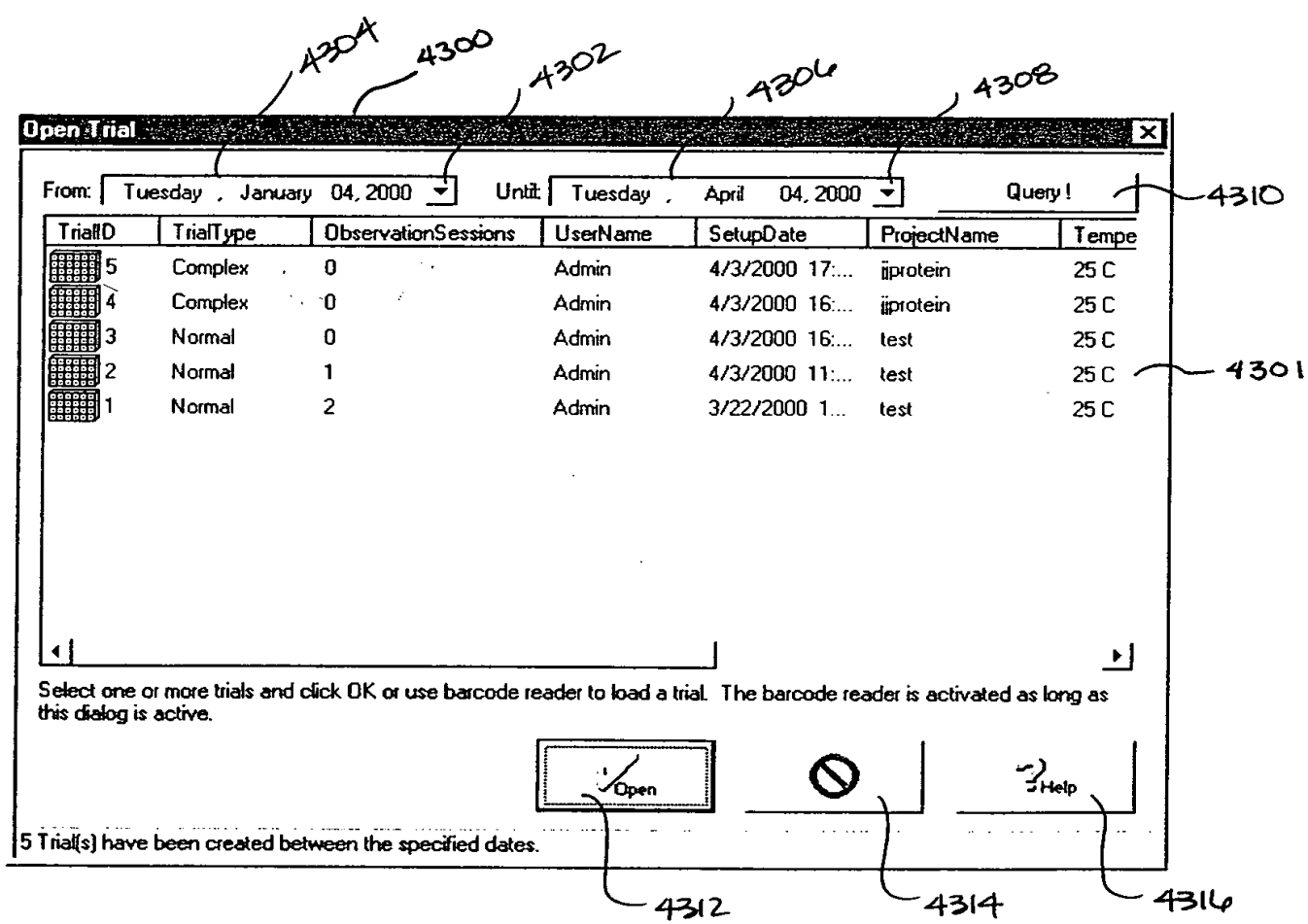


FIG. 43

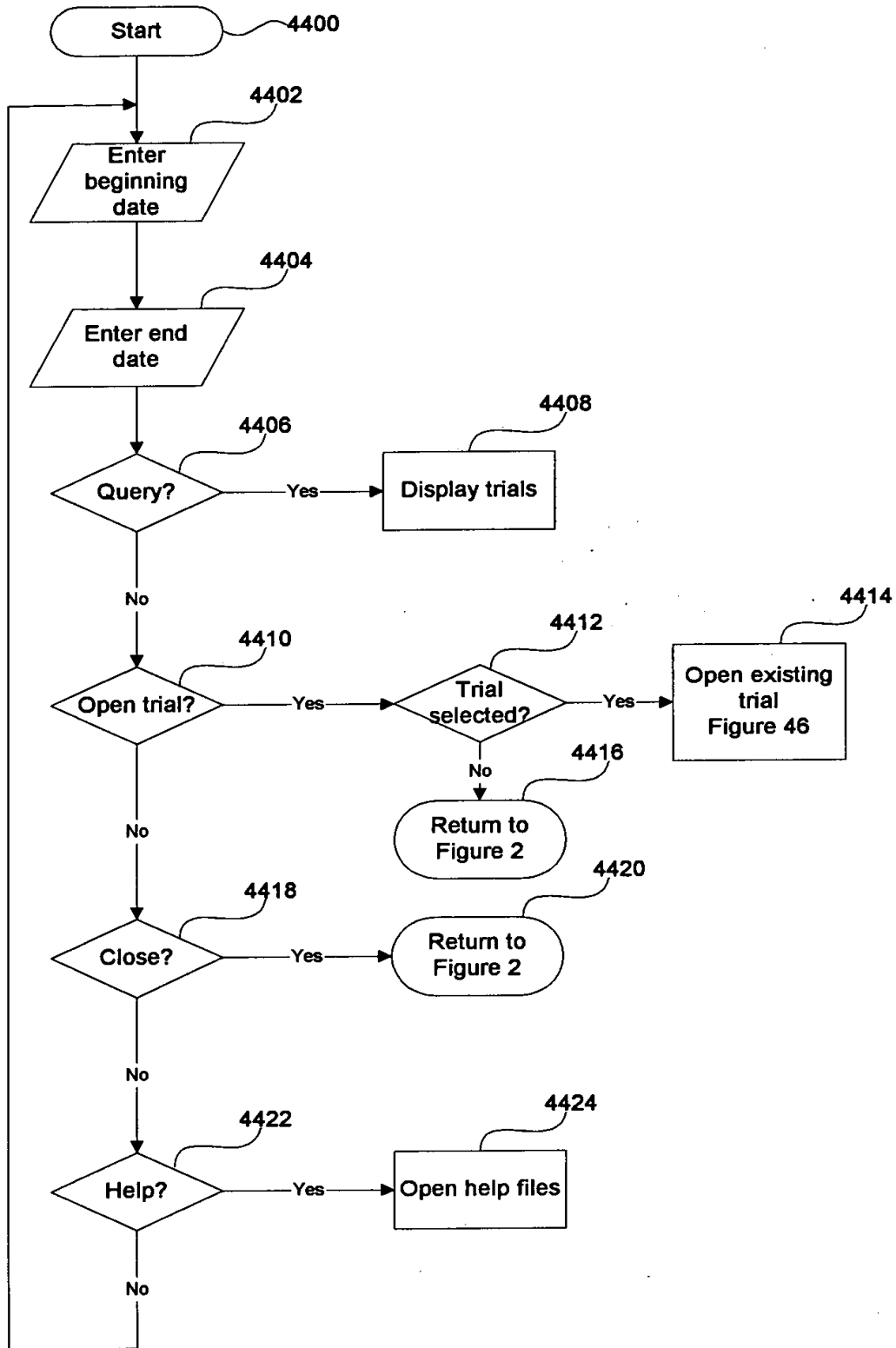


FIGURE 44

002080"58TTC960

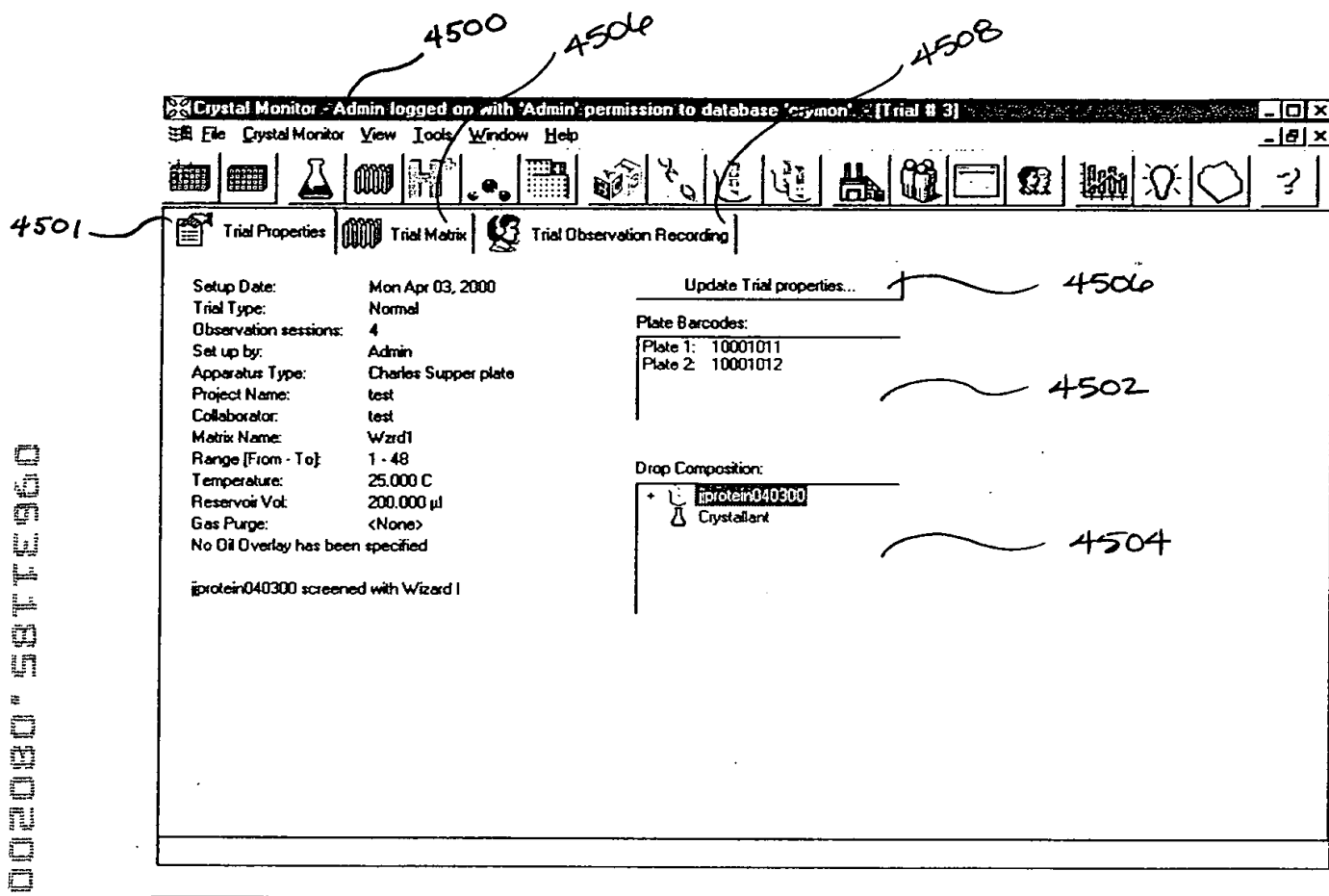


Fig. 45

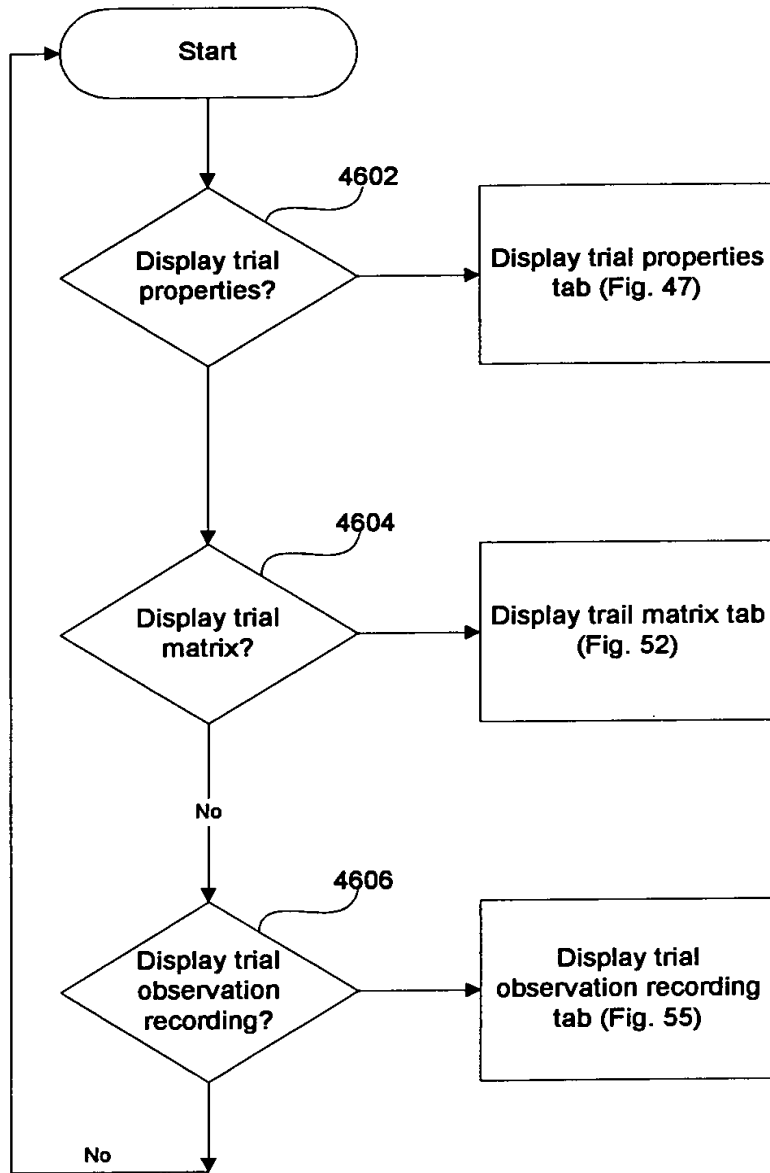
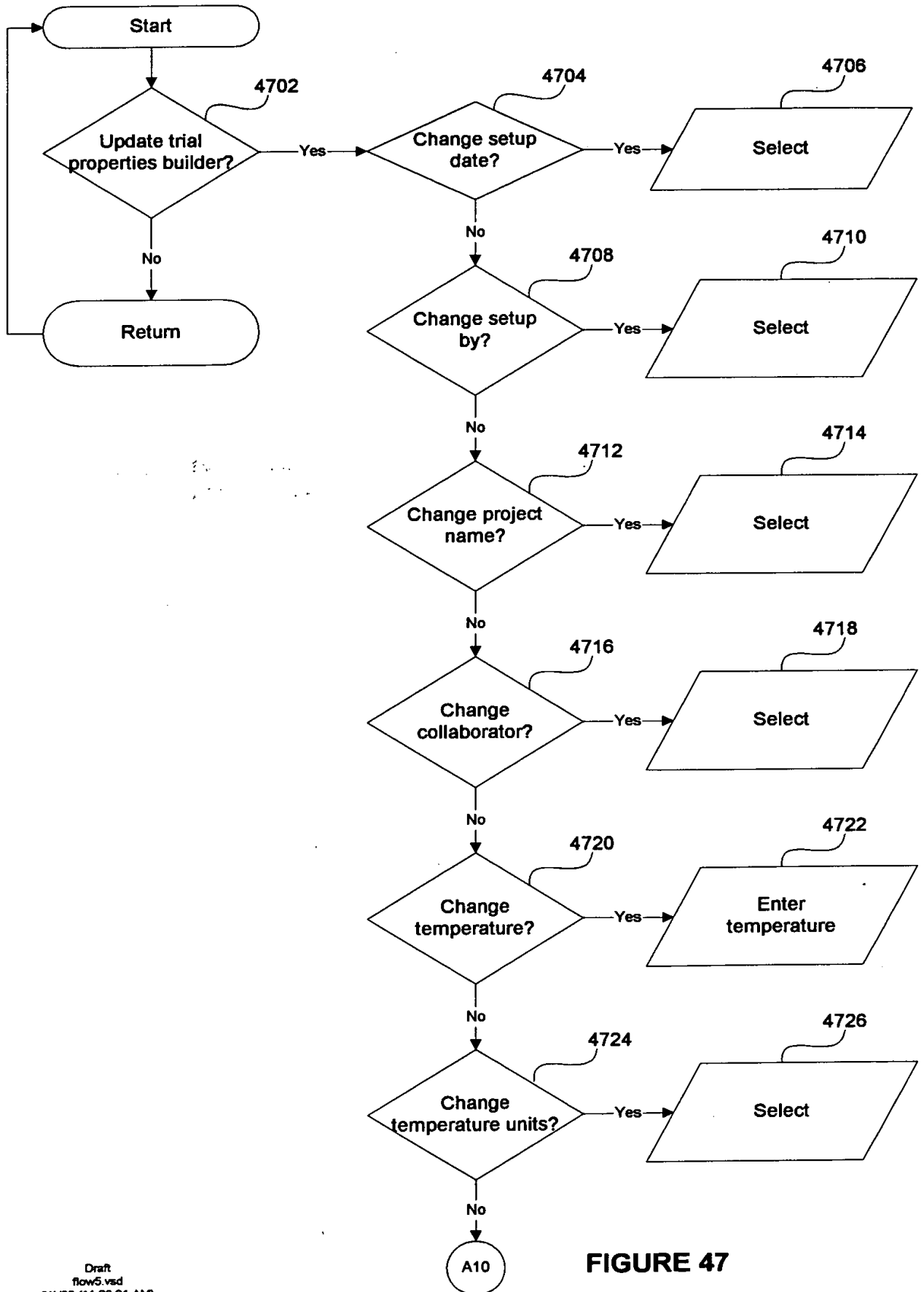


FIGURE 46



**FIGURE 47**



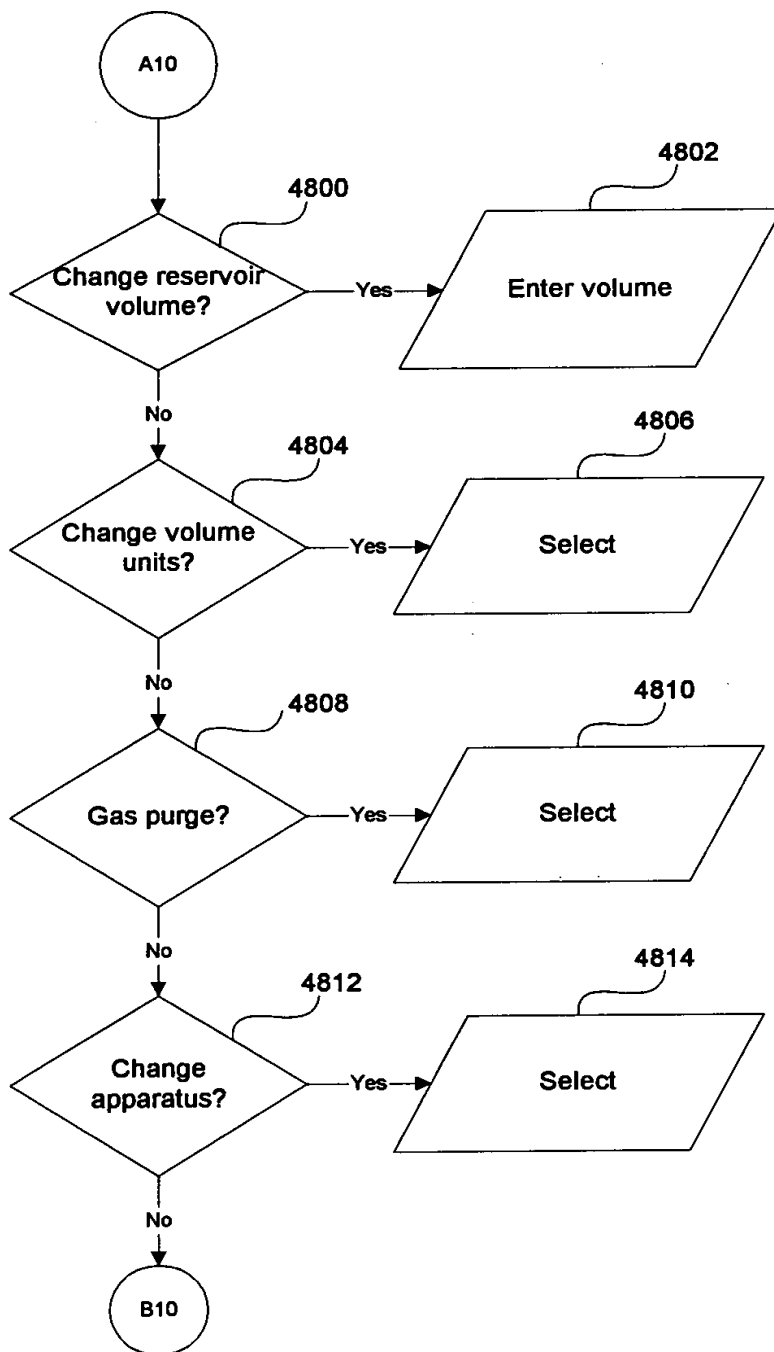
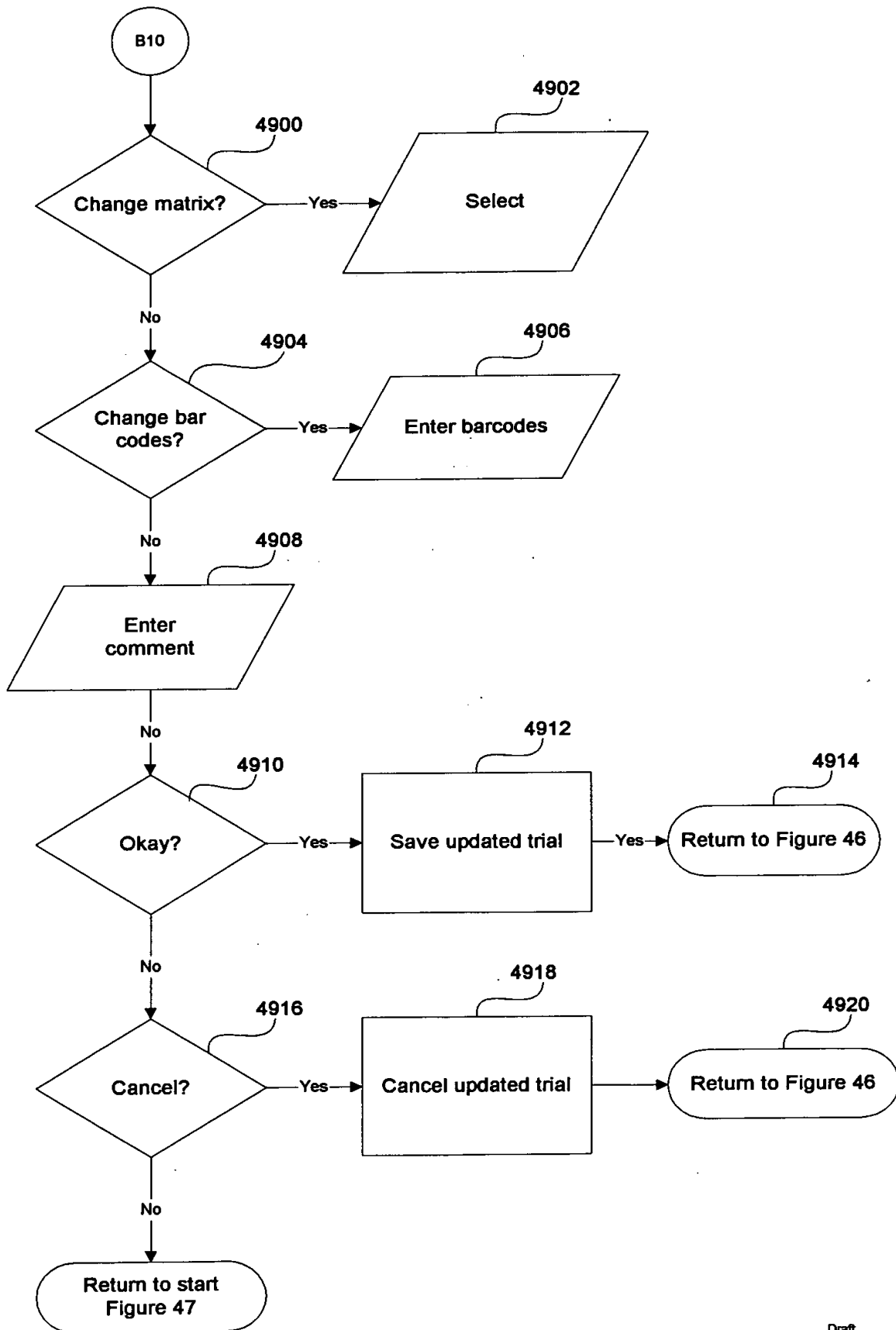


FIGURE 48



**FIGURE 49**

0963185.080200

5000

Crystal Monitor - Admin logged on with 'Admin' permission to database 'crymon'. - [Trial # 3]

File Crystal Monitor View Tools Window Help

5002

Matrix Name: Wzd1  
Matrix Type: Random  
Commercial:

- Well 8 -

Compound Buffers:  
100.000 mM (Na3 citrate, citric acid) pH 5.50

Chemicals:  
2000.000 mM (NH4)2 sulfate, Precipitant (Sigma Chemical Co. A2939)

Crystallization Drop:  
2.000 µl iprotein040300  
2.000 µl Crystallant

Solution Properties:  
Final pH: 5.50 est.  
Conductivity: n/a  
Vapor Pressure Osmolality: n/a  
Viscosity: Low  
Solvent: H2O

5004

Fig. 50

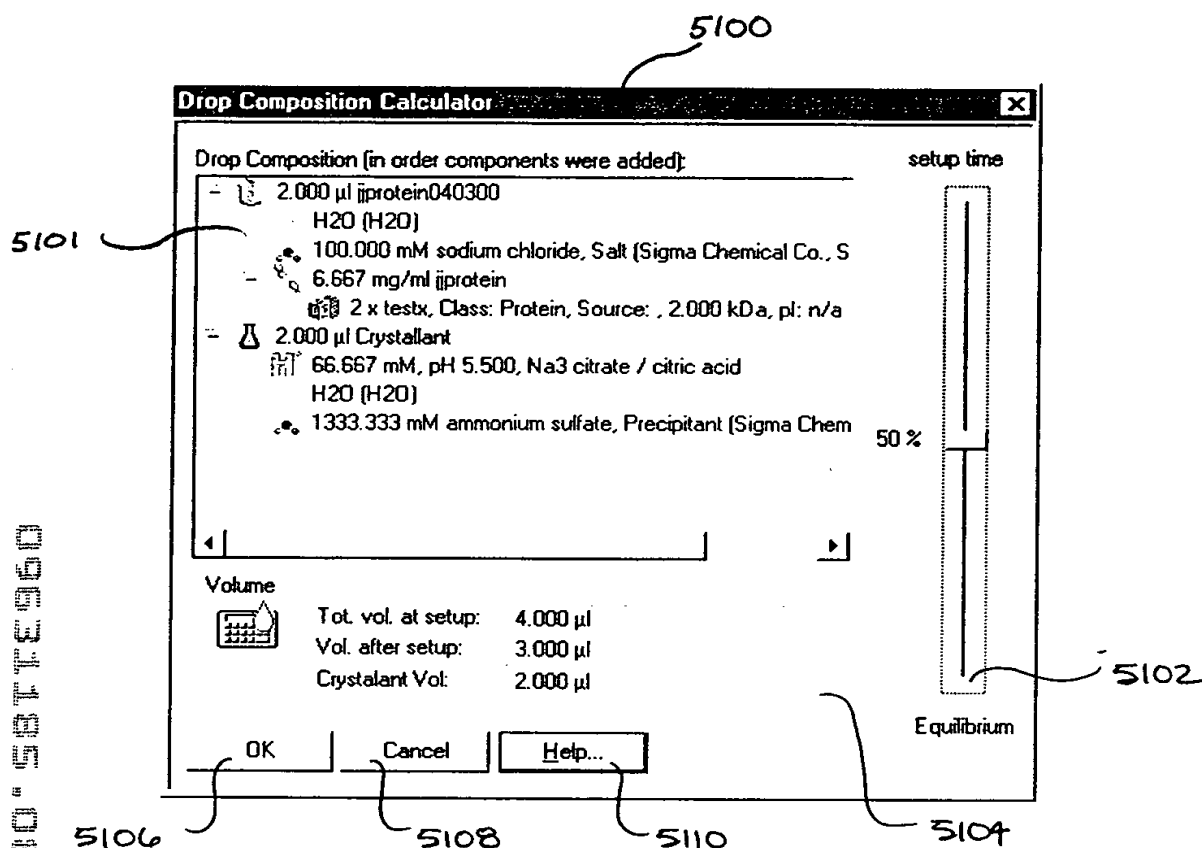


Fig. 51

```
graph TD
    Start([Start]) --> 5202[Display matrix properties]
    5202 --> 5204[Display crystallization matrix template]
    5204 --> 5206{Drop composition calculator?}
    5206 -- Yes --> 5208[Run drop composition calculator]
    5208 --> 5210
    5206 -- No --> 5210
    5210 --> 5212{Okay?}
    5212 -- Yes --> 5212_Return([Return Figure 46])
    5212 -- No --> 5214{Cancel?}
    5214 -- Yes --> 5214_Return([Return Figure 46])
    5214 -- No --> 5218{Help?}
    5218 -- Yes --> 5220[Open help files]
    5218 -- No --> 5210
```

Flowchart 5200 illustrates the process of displaying matrix properties and handling user input. The process begins with a 'Start' terminal, leading to a process block 'Display matrix properties' (5202). This is followed by 'Display crystallization matrix template' (5204). A decision diamond 'Drop composition calculator?' (5206) follows. If 'Yes', the process proceeds to 'Run drop composition calculator' (5208). If 'No', the process bypasses 5208 and proceeds to a junction point before decision diamond 'Okay?' (5212). From 'Okay?' (5212), a 'Yes' response leads to 'Return Figure 46' (5212), and a 'No' response leads to decision diamond 'Cancel?' (5214). From 'Cancel?' (5214), a 'Yes' response leads to 'Return Figure 46' (5214), and a 'No' response leads to decision diamond 'Help?' (5218). From 'Help?' (5218), a 'Yes' response leads to 'Open help files' (5220), and a 'No' response loops back to the junction point before 'Okay?' (5212).

Draft  
flow5.vsd  
07/31/2000 (6:52:21 PM)

002080 "587E960

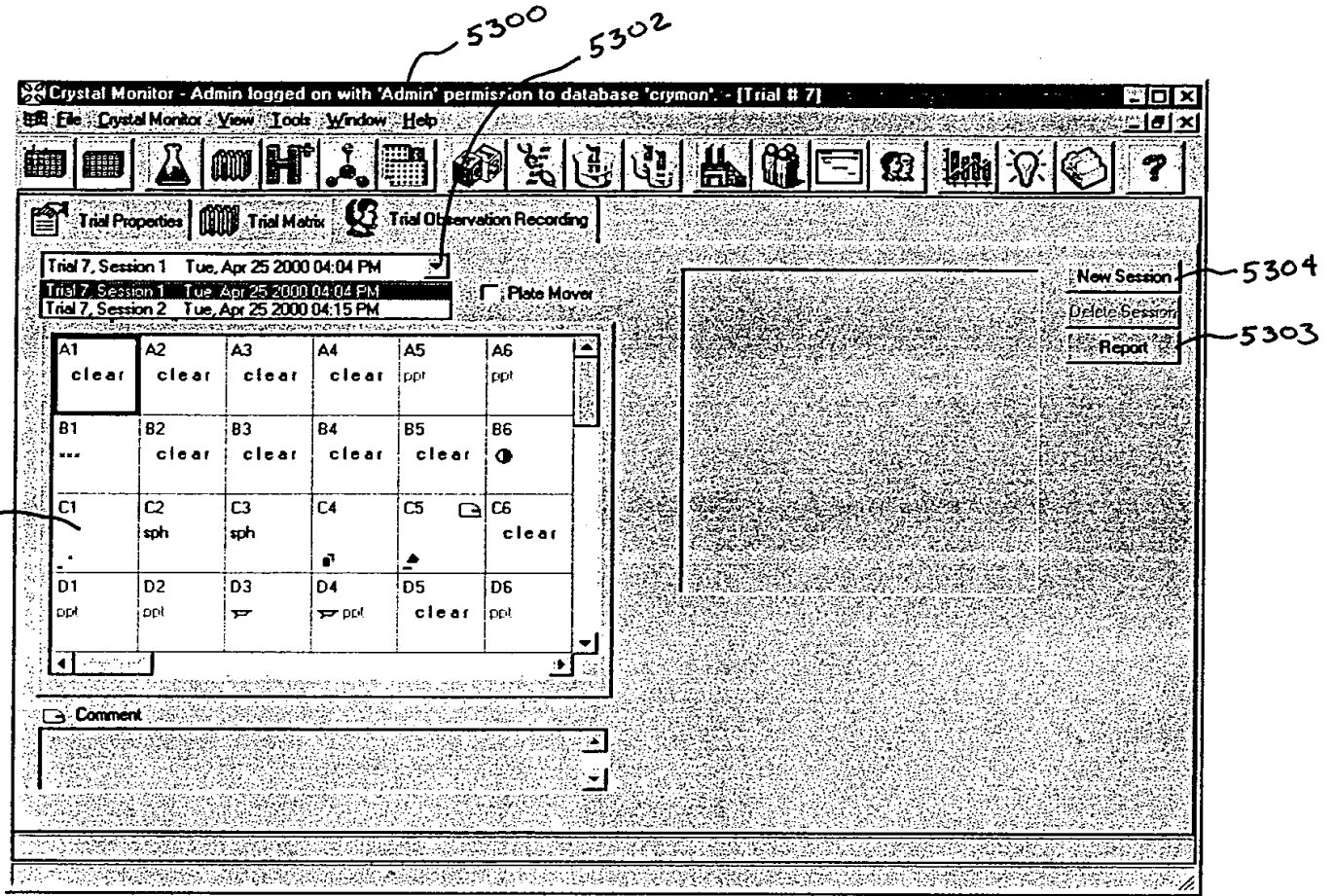


Fig. 53

0963185-080200

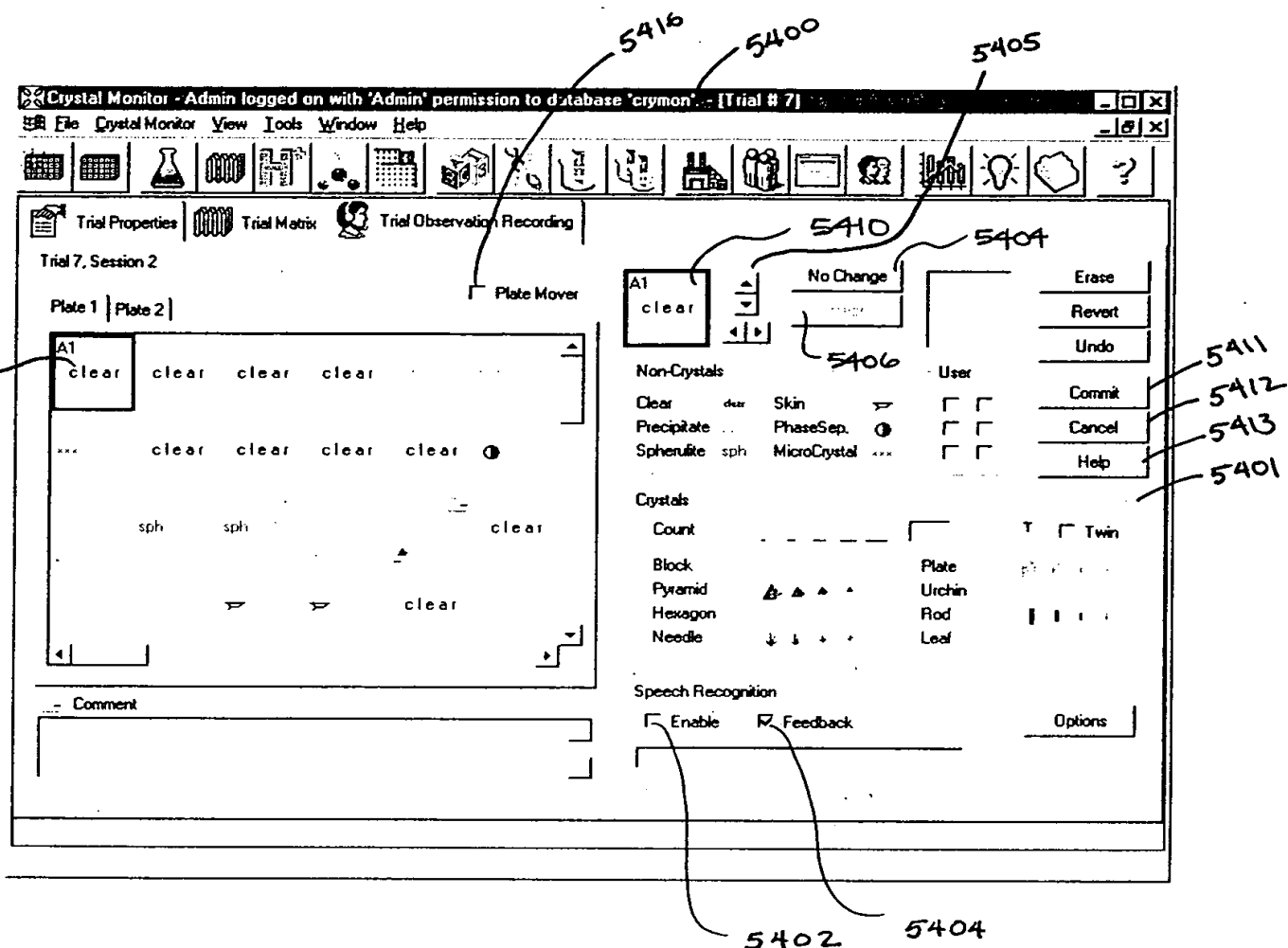


Fig. 54

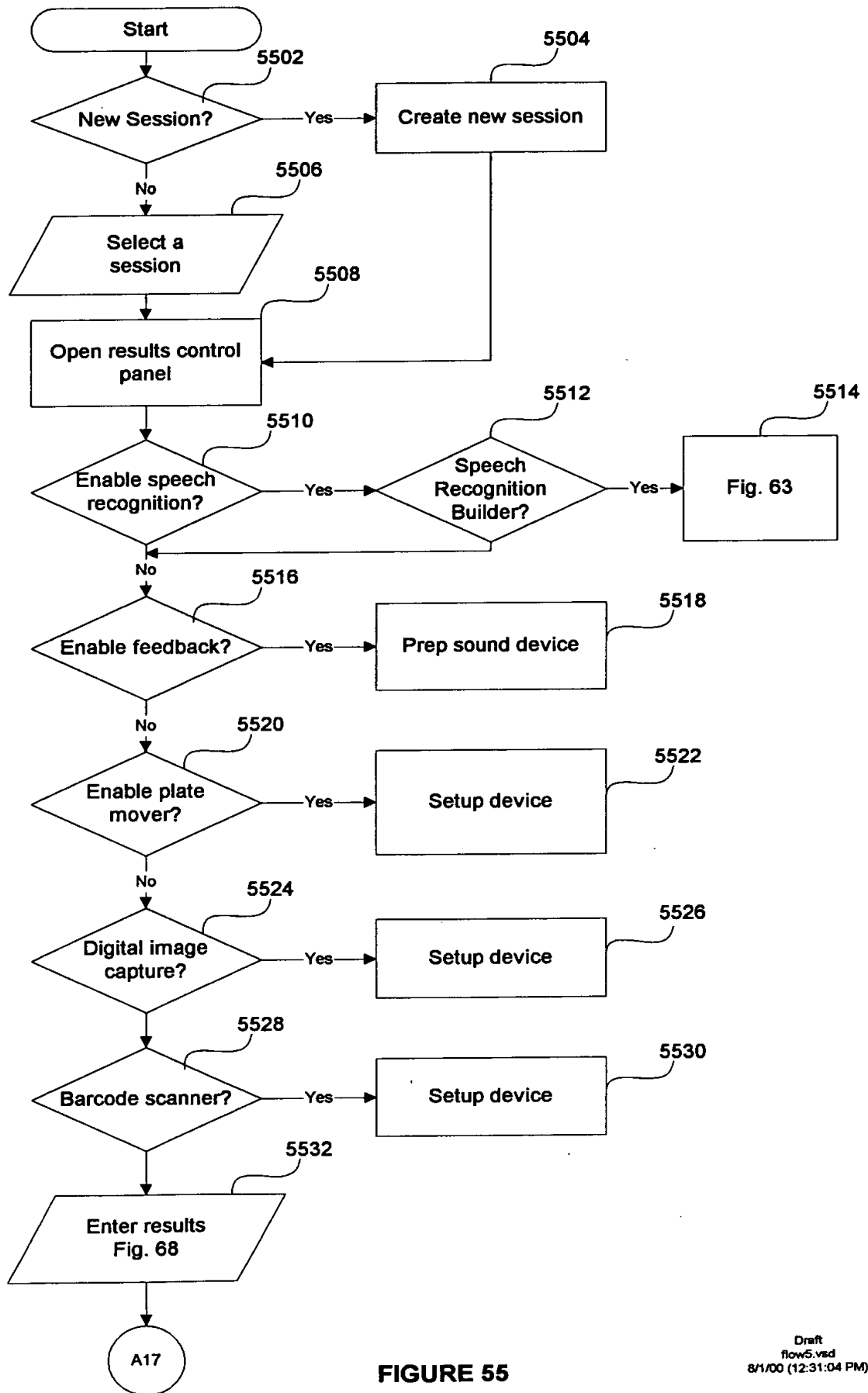


FIGURE 55



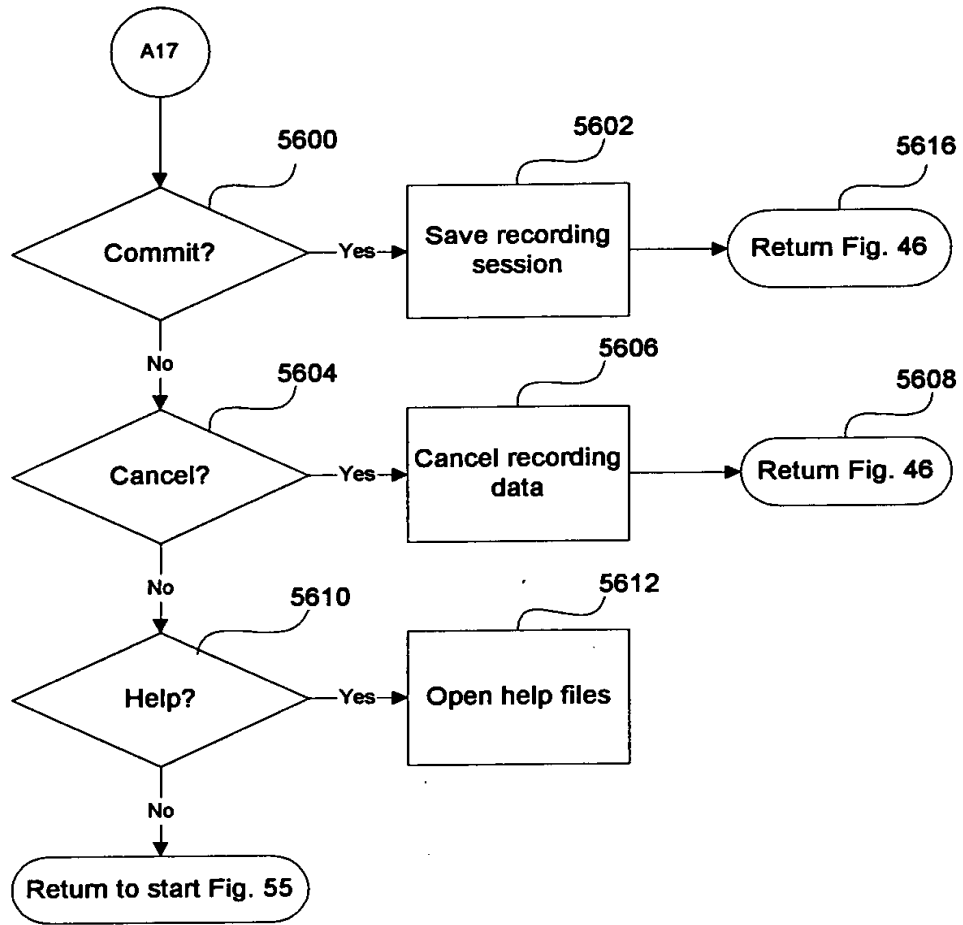
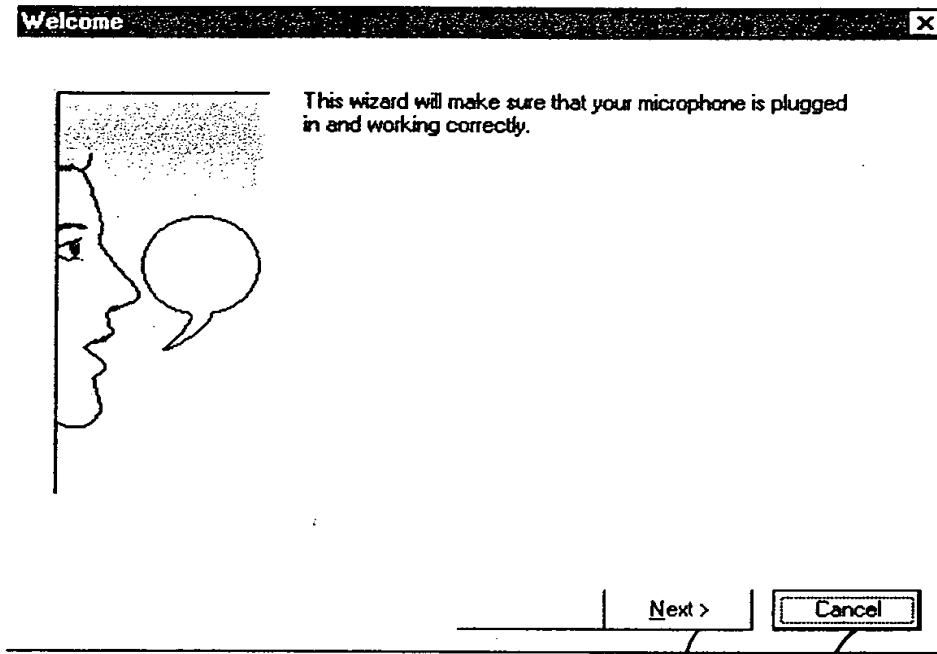


FIGURE 56

002080" 58T E960



← 5700

FIG. 57

5702

5704

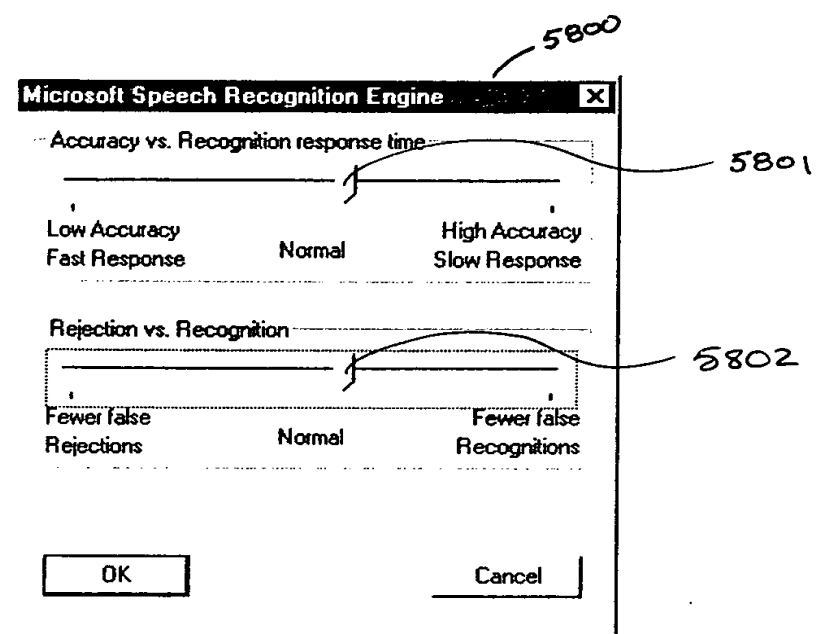


Fig. 58

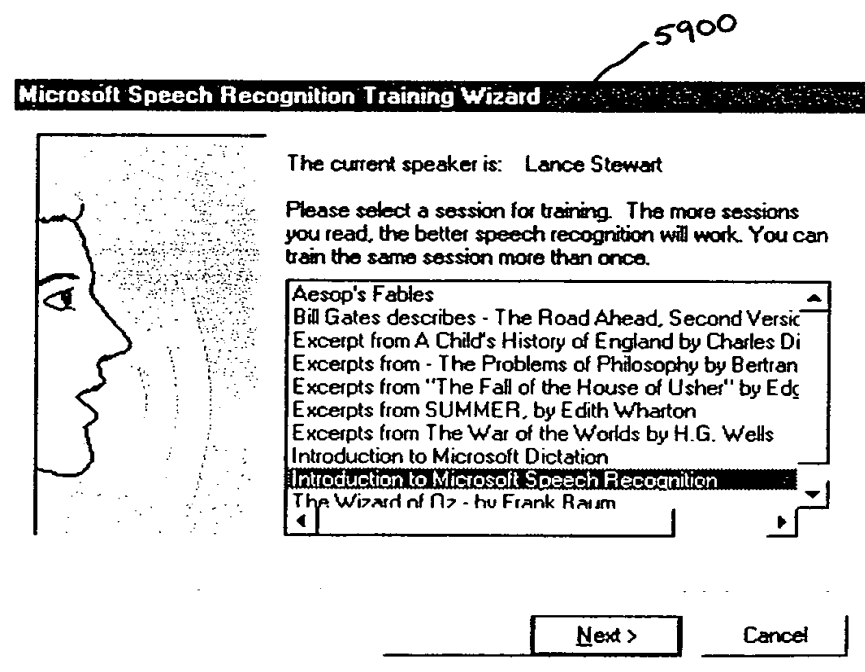


Fig. 59

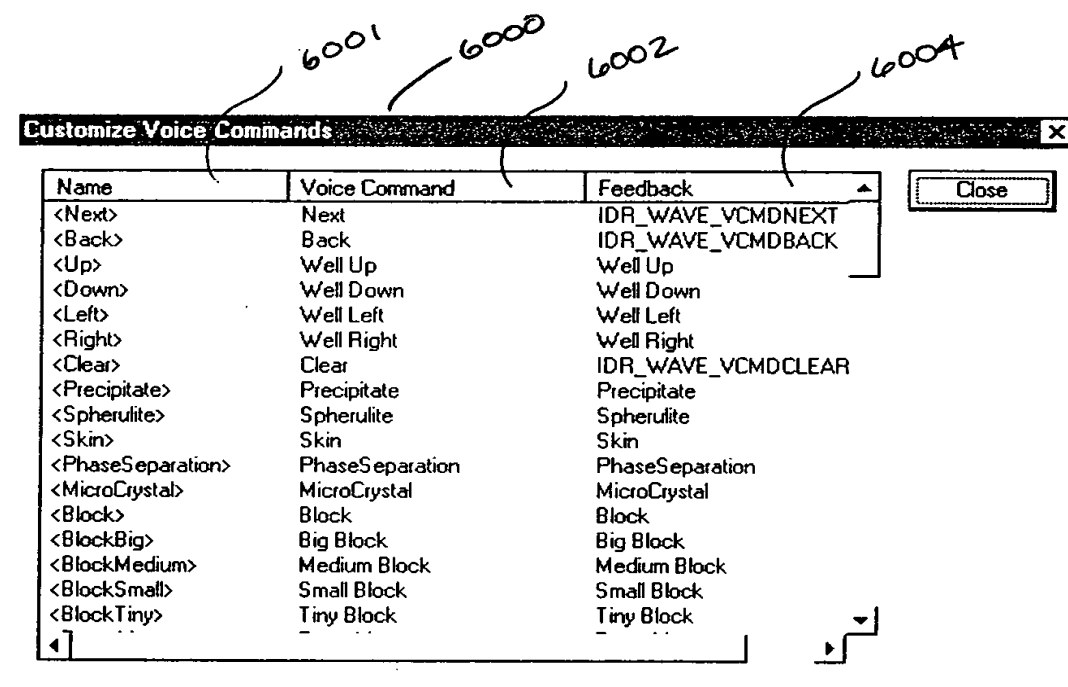


Fig. 60

0963185.080200

6100

6101

6105

6106

6102

6104

Voice Command

Name

<Clear>

OK

Cancel

Voice Command

Clear

Feedback

IDR\_WAVE\_VCMDCLEAR

Fig. 61

6200

Customize Voice Commands

Name	Voice Command	Feedback
<Down>	Well Down	Well Down
<Left>	Well Left	Well Left
<Right>	Well Right	Well Right
<FirstWell>	First Well	First Well
<LastWell>	Last Well	Last Well
<Clear>	clear	IDR_WAVE_VCMDCLEAR
<Precipitate>	Precipitate	Precipitate
<Spherulite>	Spherulite	Spherulite
<Skin>	Skin	Skin
<PhaseSeparation>	PhaseSeparation	PhaseSeparation
<MicroCrystal>	MicroCrystal	MicroCrystal
<User1>	flocculent	flocculent
<User2>	heavy	heavy
<User3>	granular	granular
<Block>	Block	Block
<BlockBig>	Big Block	Big Block
<BlockMedium>	Medium Block	Medium Block

Close

Edit..

FIG. 62

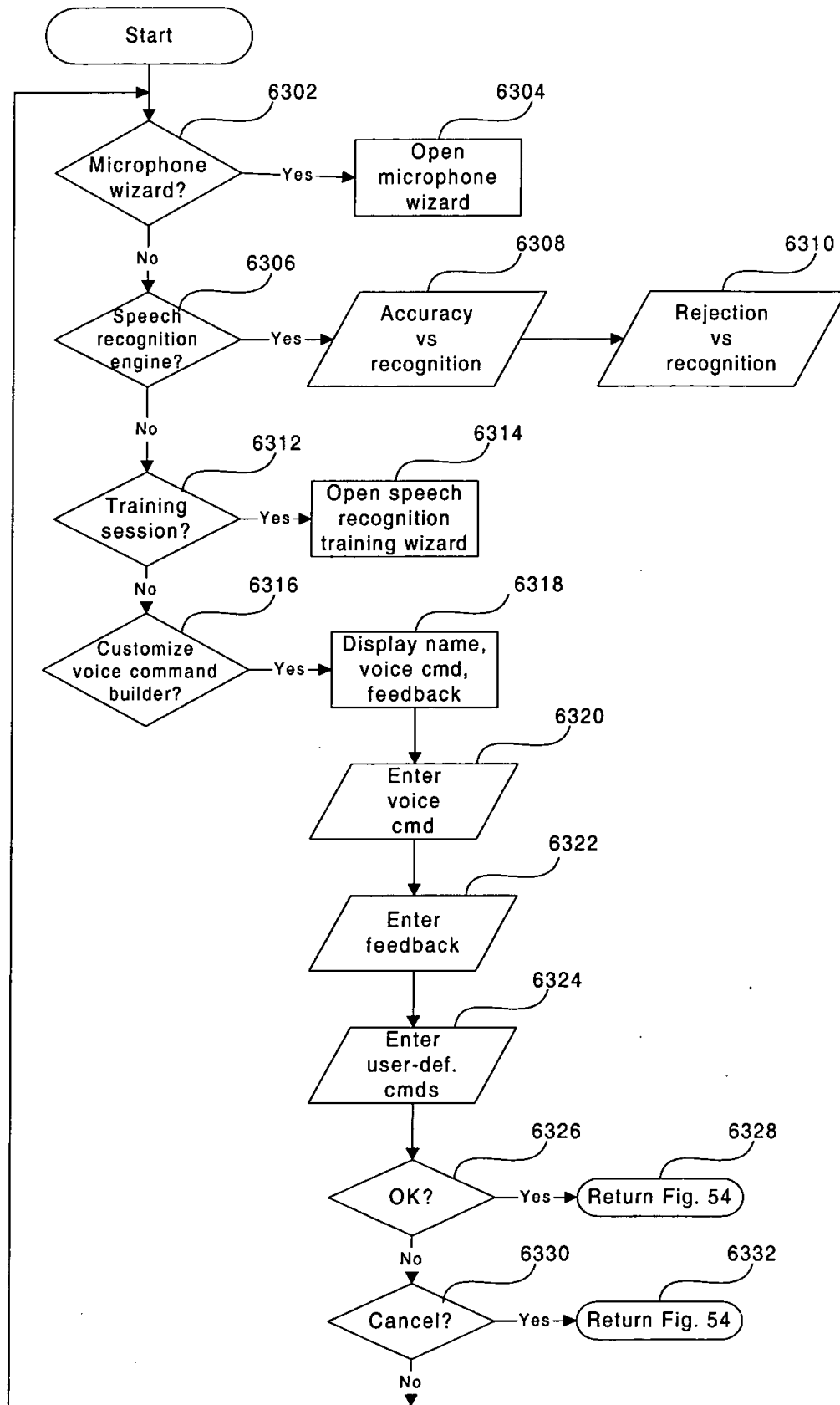
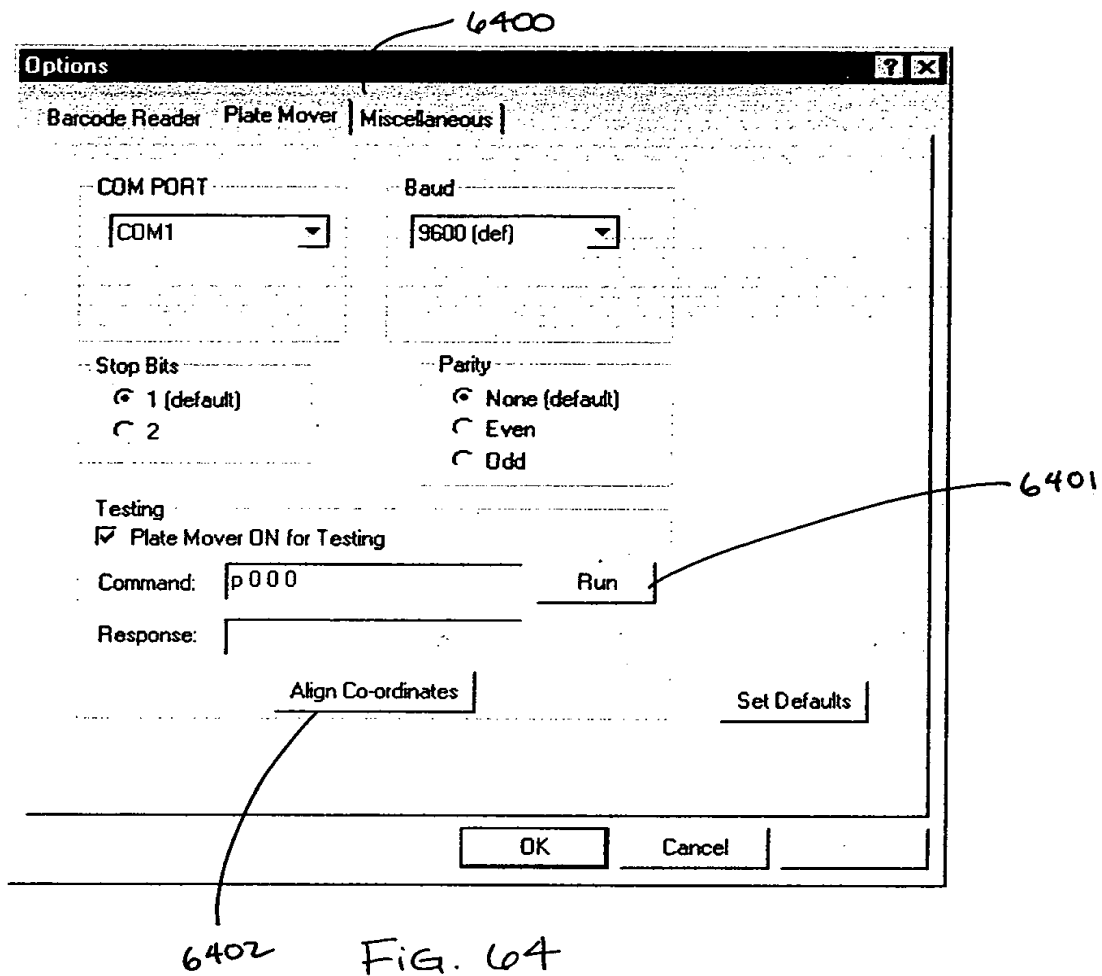


FIGURE 63

002080"58TTC960





002080"58TFE960

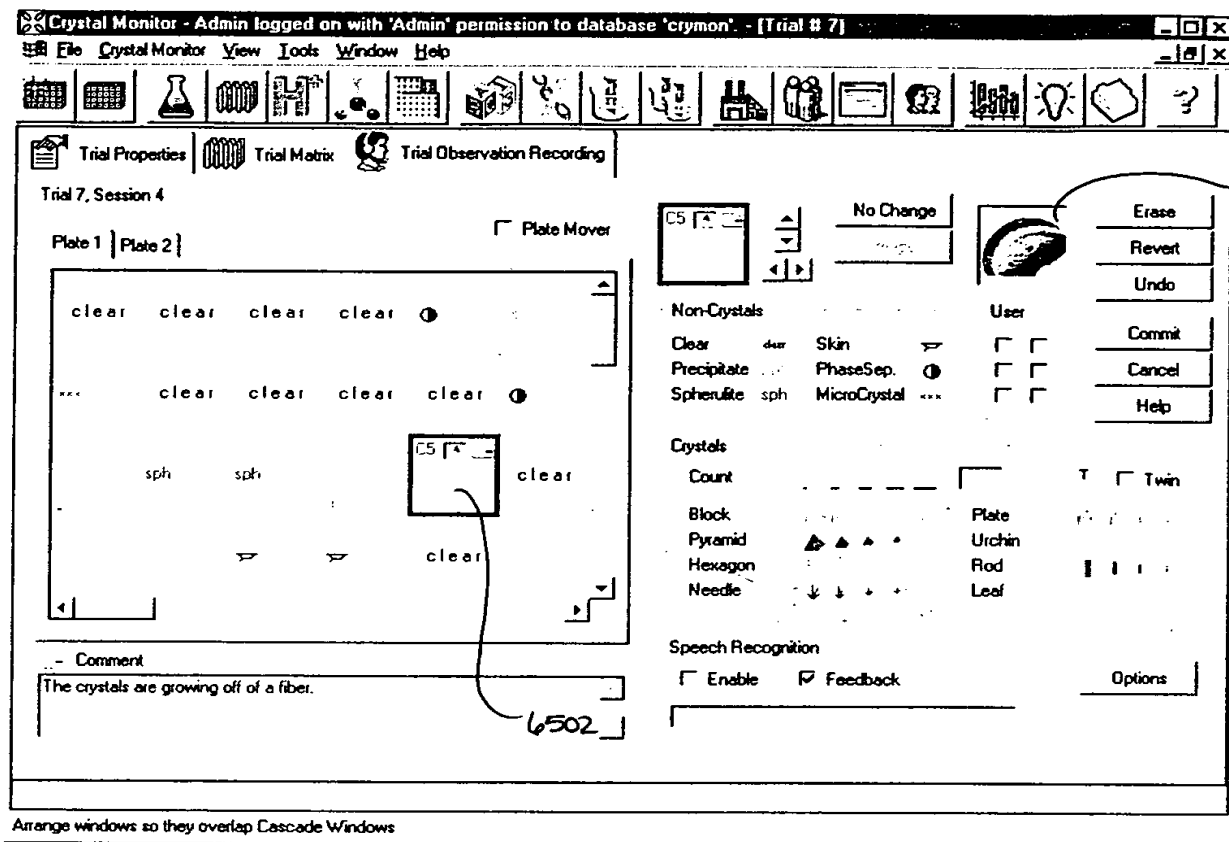


FIG. 65

003030" SET E 960

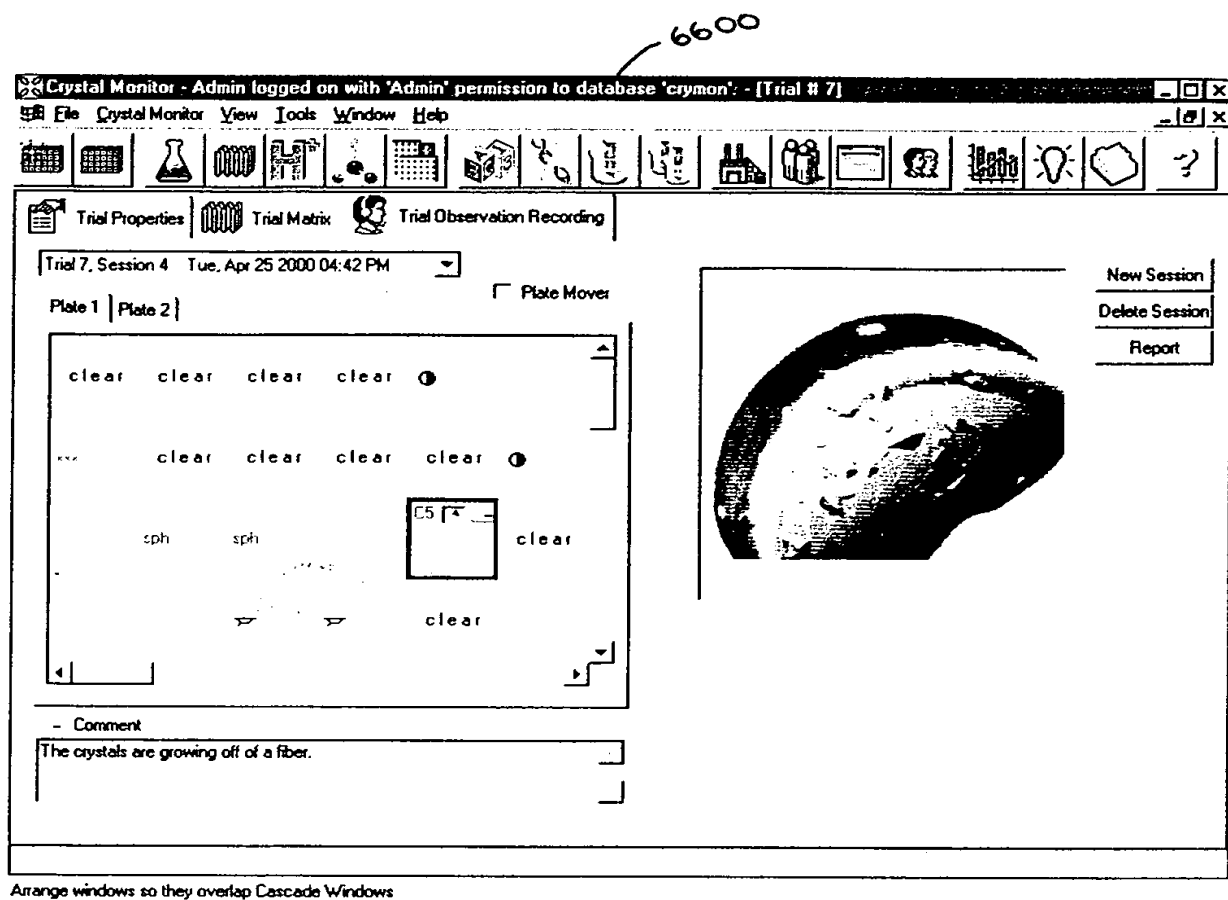


FIG. 66

002080 587E960

6700

**Options** ? X

Barcode Reader | Plate Mover | Miscellaneous |

COM PORT: COM1

Baud: 9600 (def)

Stop Bits: ☒ 1 (default) ☐ 2

Parity: ☒ None (default) ☐ Even ☐ Odd

Testing: ☒ Barcode Reader ON for Testing

Scanned Barcode: \_\_\_\_\_

Set Defaults

OK Cancel

Fig. 67

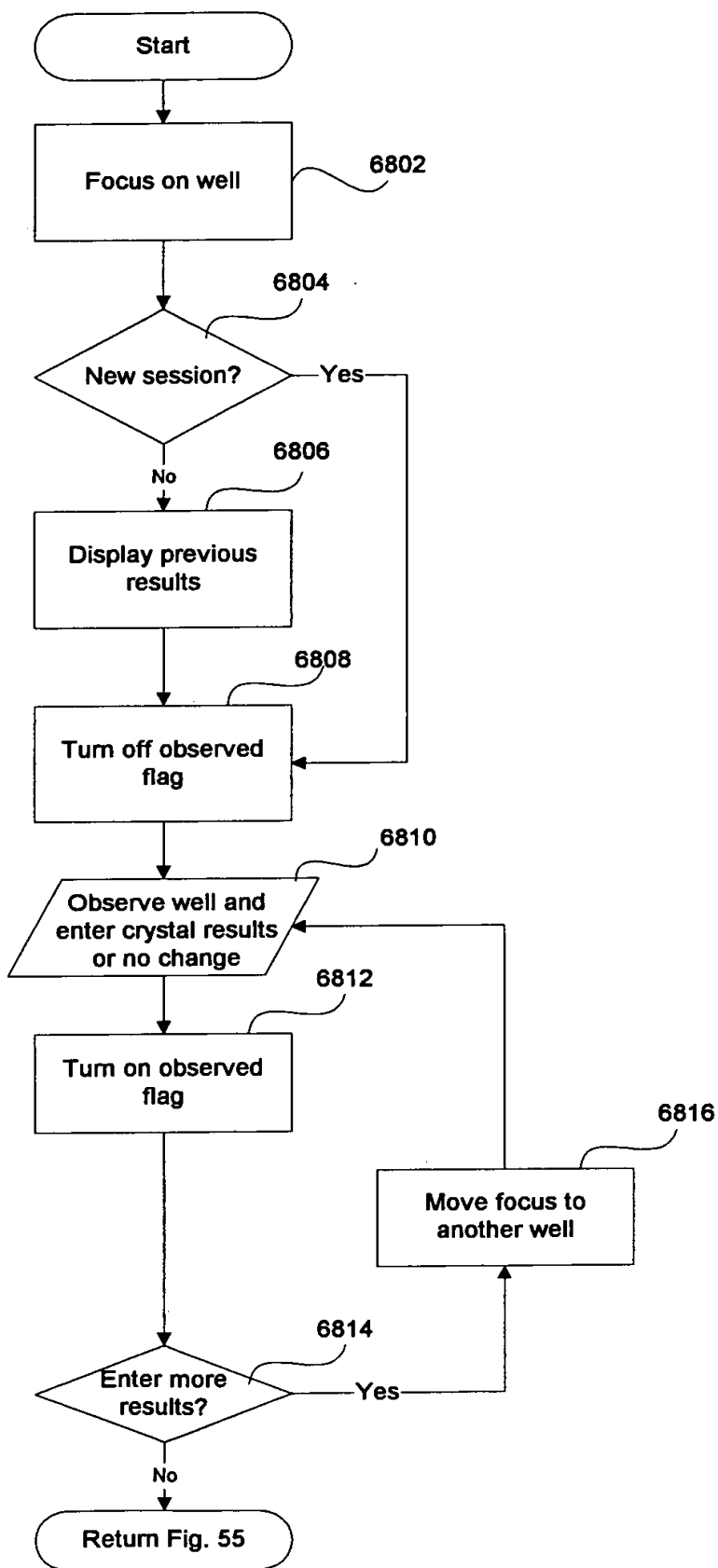


FIGURE 68

09631185-080200


clear clear clear clear ●  
xxx clear clear clear clear ●  
sph sph CS  clear  
clear

Fig. 69

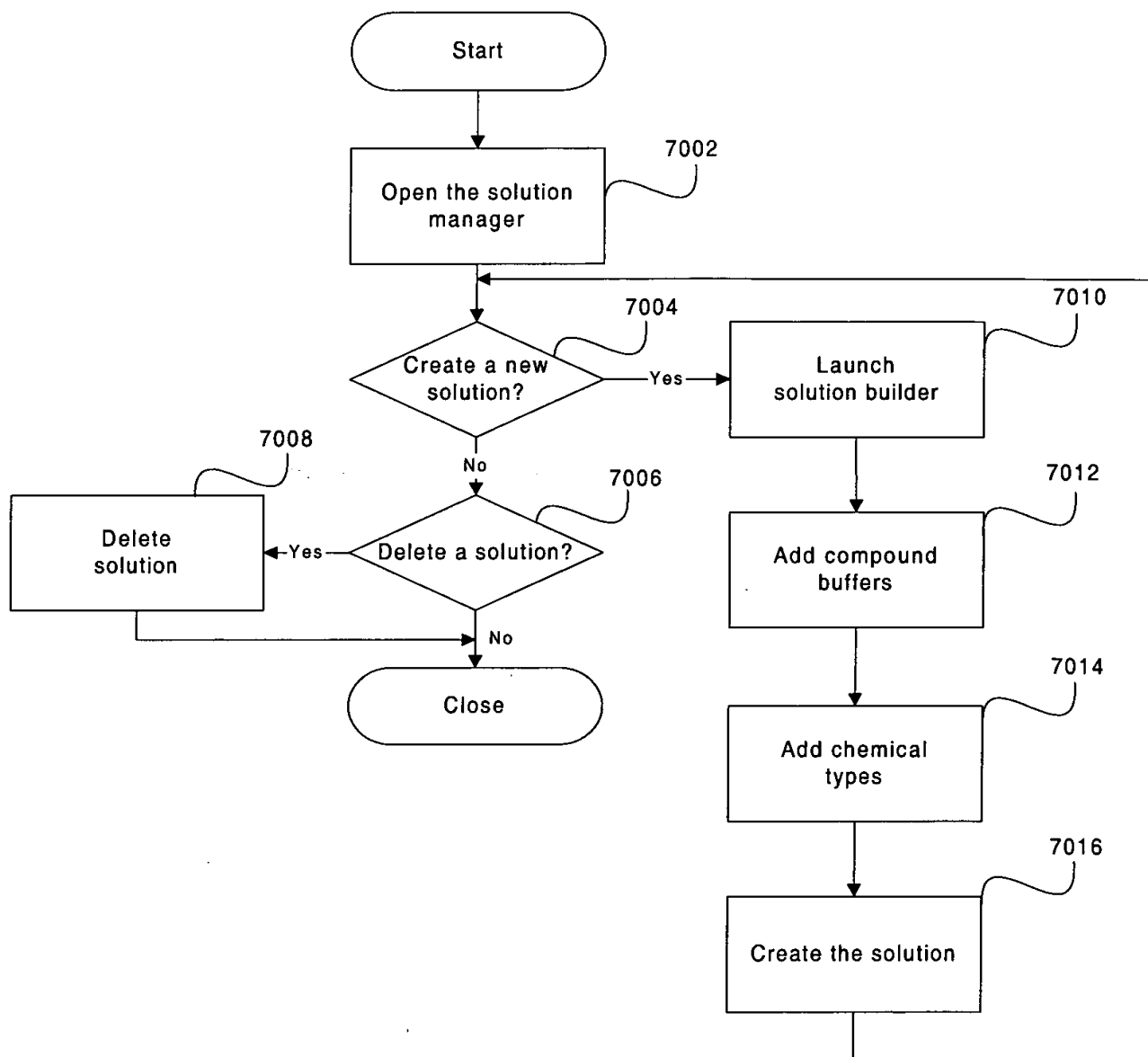
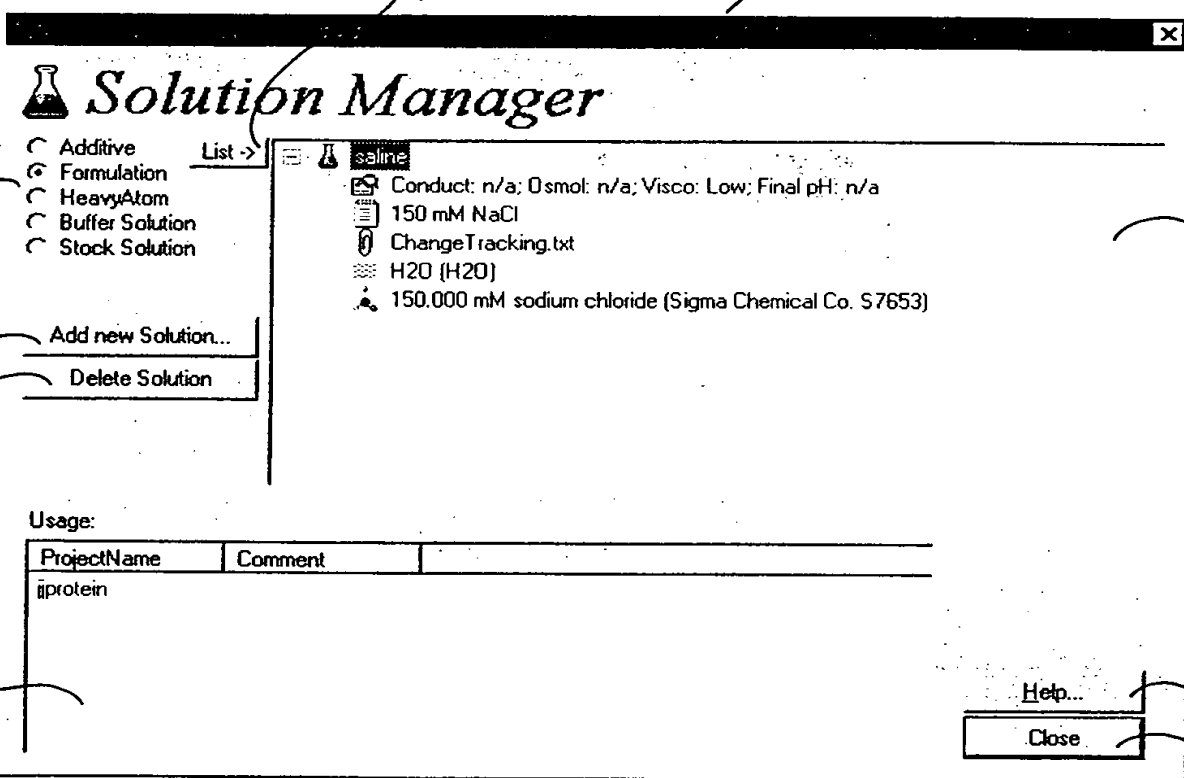


FIGURE 70



44

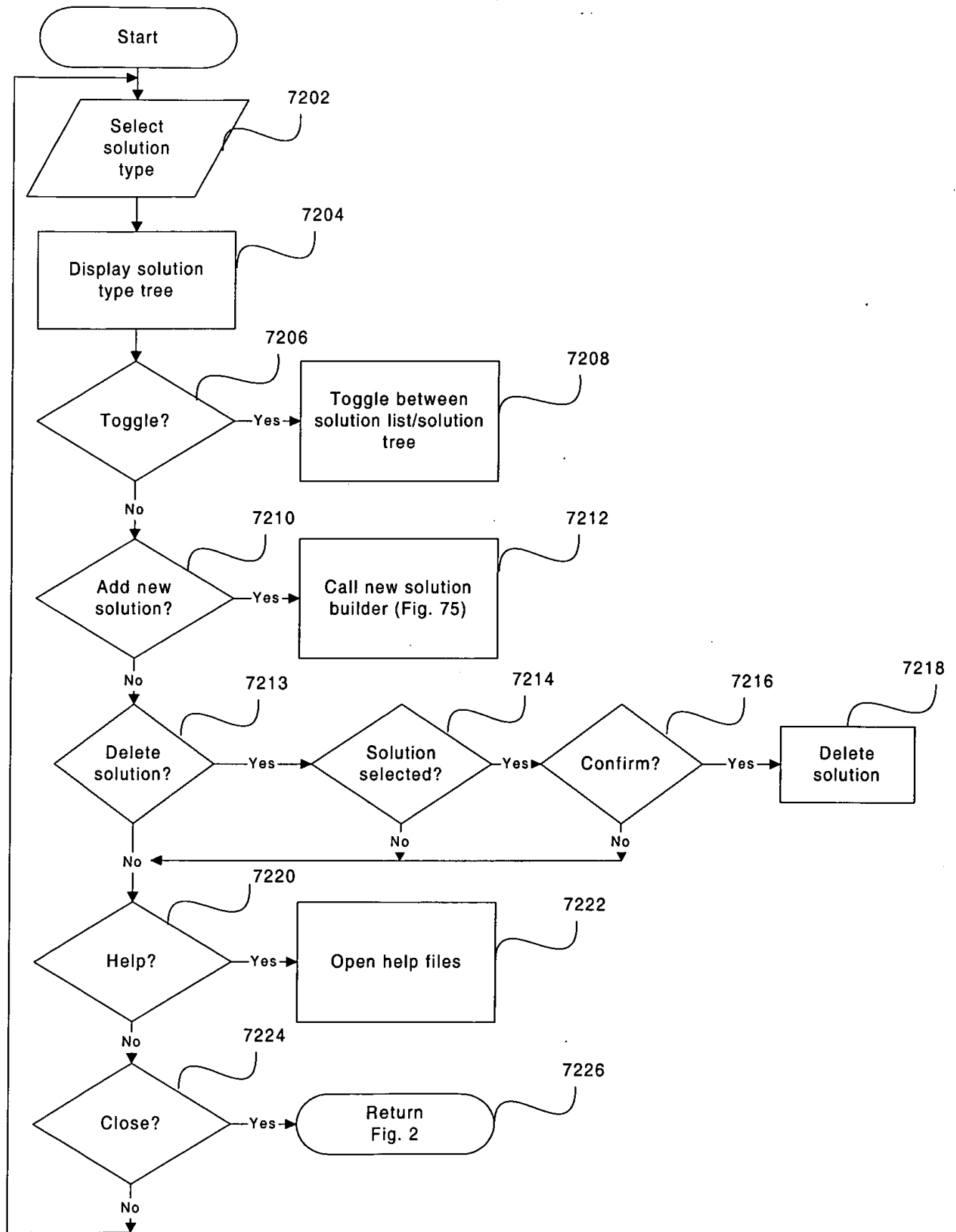


FIGURE 72



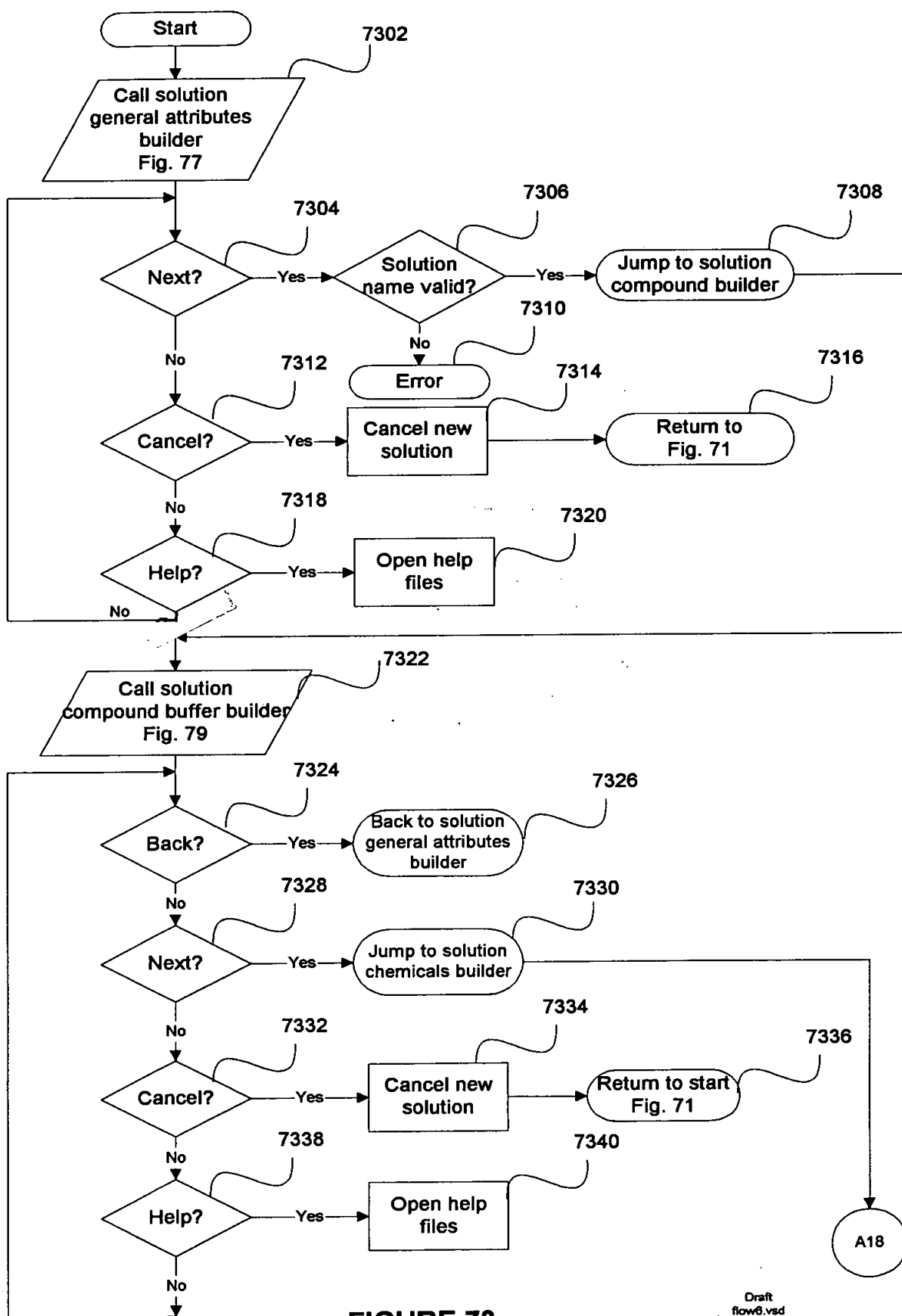


FIGURE 73

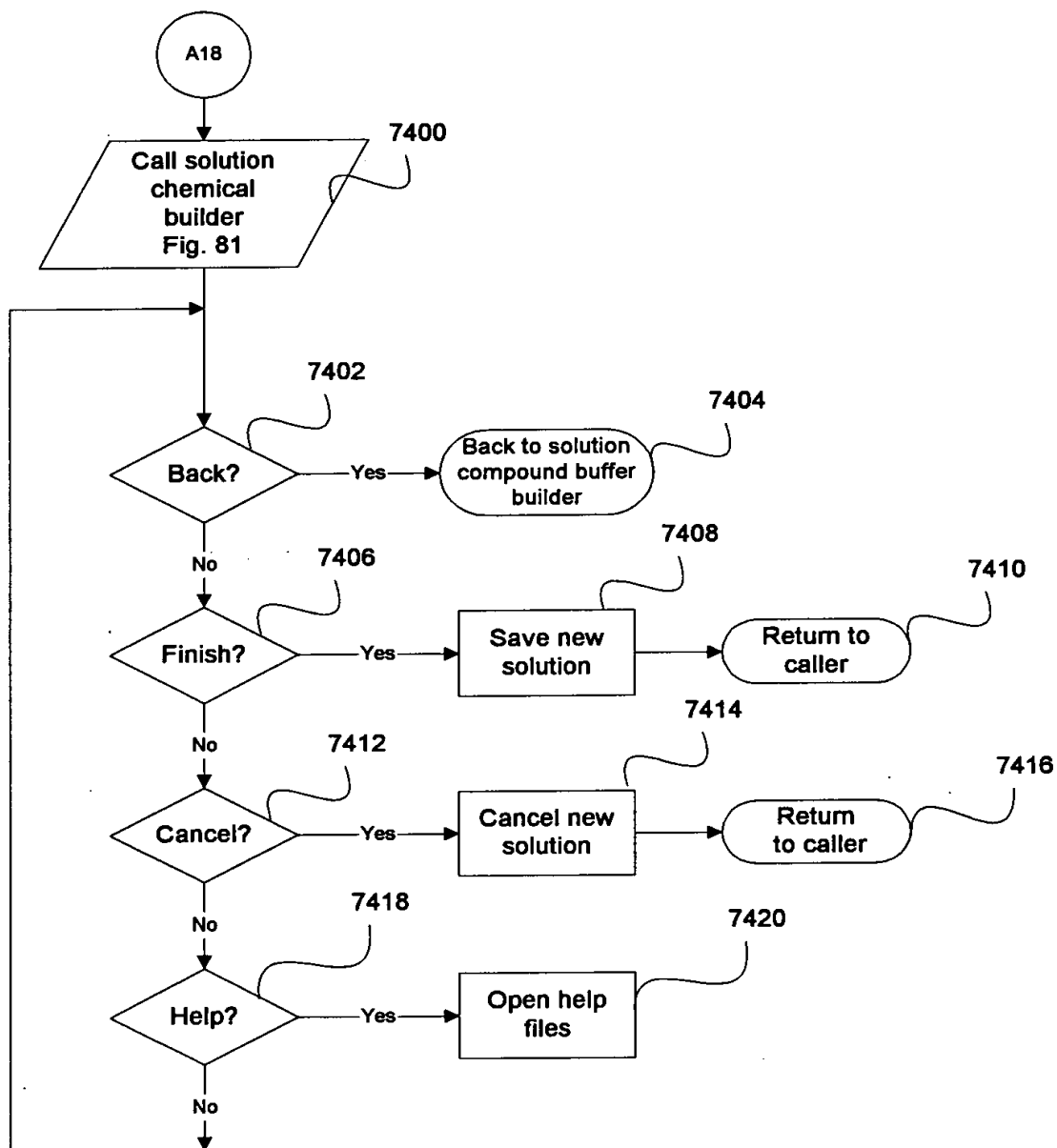


FIGURE 74

**Solution Wizard - General**

**Solution Type**

- ☐ Additive
- ☒ Formulation
- ☐ Heavy Atom
- ☐ Buffer Solution
- ☐ Stock Solution

**pH of Solution**

- ☒ Estimated
- ☐ Measured

**Viscosity**

- ☒ Low
- ☐ High

**Solution Attributes**

pH of Solution:

Vapor Pressure Osmolality:  mmole/kg

Conductivity:   $\mu\text{S}/\text{cm}$

Solvent:  H2O (Mothé)

Solution Name:  ammsulf040400

**Comment**

200 mM ammonium sulfate 100 mM Tris pH 7.0

**Buttons:** < Back, Next >, Cancel, Help

**Image:** A small image of several vials is located in the top left corner of the dialog box.

**Reference Numerals:**

- 7500: Title bar
- 7502: Solution Type group box
- 7502: pH of Solution group box
- 7504: Estimated radio button
- 7508: Viscosity group box
- 7506: Low radio button
- 7512: pH of Solution text field
- 7518: Vapor Pressure Osmolality text field
- 7510: mmole/kg unit
- 7516: Conductivity text field
- 7514:  $\mu\text{S}/\text{cm}$  unit
- 7528: Solvent text field
- 7524: H2O (Mothé) solvent selection
- 7526: Solution Name text field
- 7522: ammsulf040400 solution name
- 7531: Comment text field
- 7530: 200 mM ammonium sulfate 100 mM Tris pH 7.0 comment
- 7532: < Back button
- 7534: Next > button
- 7536: Cancel button
- 7538: Help button

Fig. 75

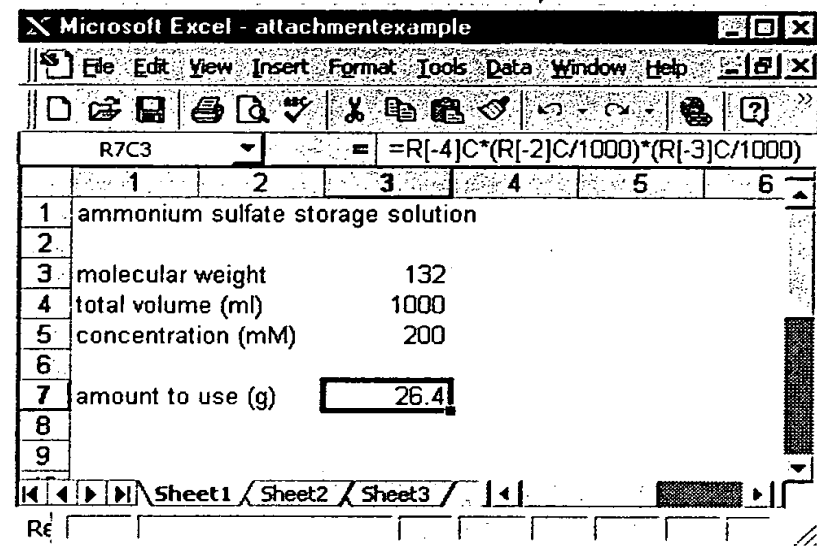


FIG. 76

002080" 5877E960

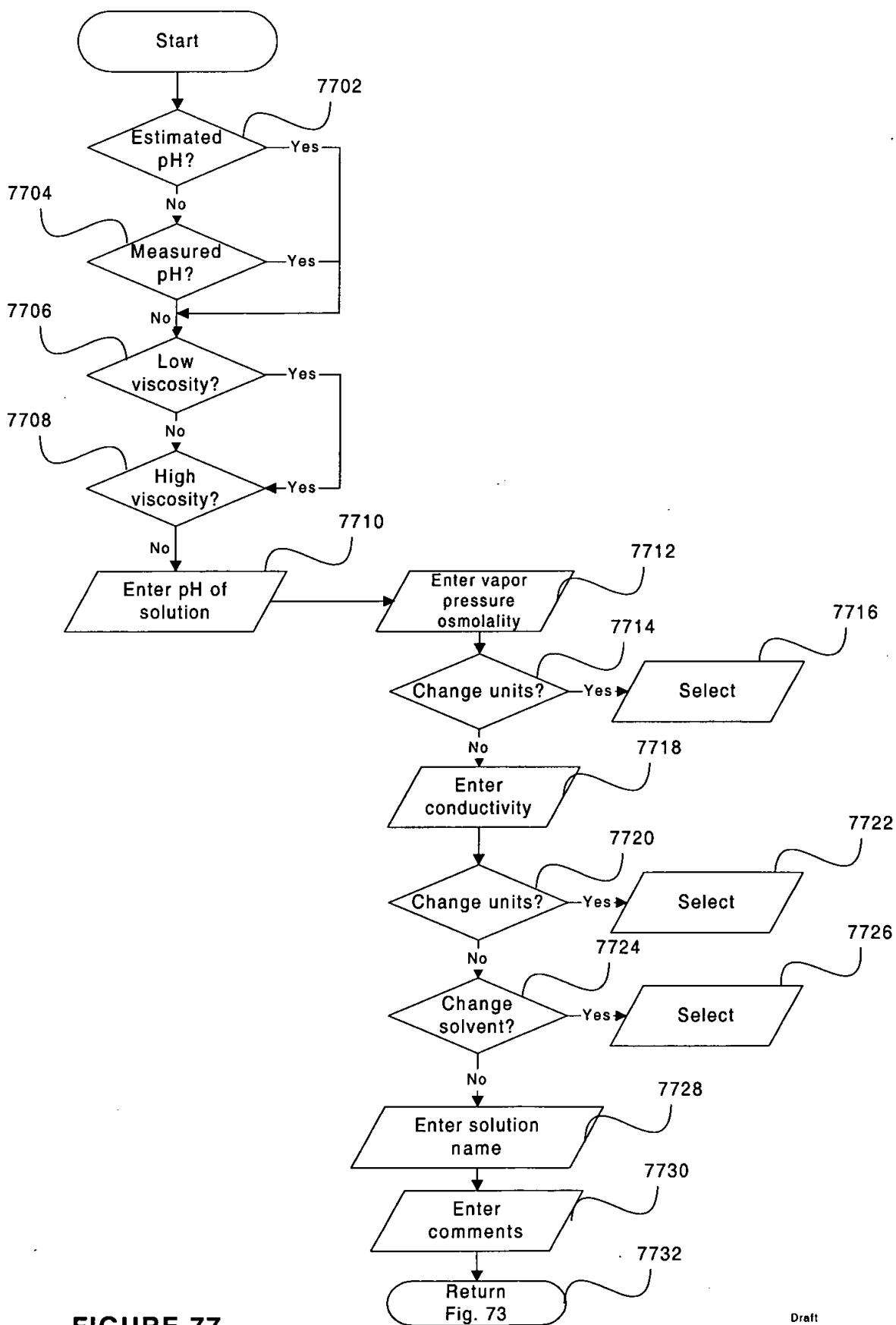


FIGURE 77

7800

Formulation: ammsulf040400

Compound Buffer Source List

Buffer PH	Buffering Agent	pH Conjugate	Comme
6.50	sodium cacodylic acid trihydr...	hydrochloric acid (HCl)	Na cac
6.50	2-morpholinoethanesulfonic a...	sodium hydroxide (NaOH)	MES-N
7.00	1,3-diaza-2,4-cyclopentadien...	hydrochloric acid (HCl)	imidazc
7.00	sodium cacodylic acid trihydr...	hydrochloric acid (HCl)	Na cac
7.00	4-(2-hydroxyethyl)piperazine-1...	sodium hydroxide (NaOH)	HEPES
7.00	tris(hydroxymethyl)aminometh...	hydrochloric acid (HCl)	Tris-HCl
7.50	N-(2-hydroxyethyl)piperazine...	sodium hydroxide (NaOH)	HEPES
7.50	4-(2-hydroxyethyl)piperazine-1...	sodium hydroxide (NaOH)	HEPES

7801

Solution Buffer List

Add Remove

Buffer PH	Concentration	Buffering Agent	pH Conjugate	Commer
7.00	100.000 mM	tris(hydroxymethyl)am...	hydrochloric acid (HCl)	Tris-HCl

7804

7806

7802

< Back Next > Cancel Help

7808

7810

7812

7814

FIG. 78

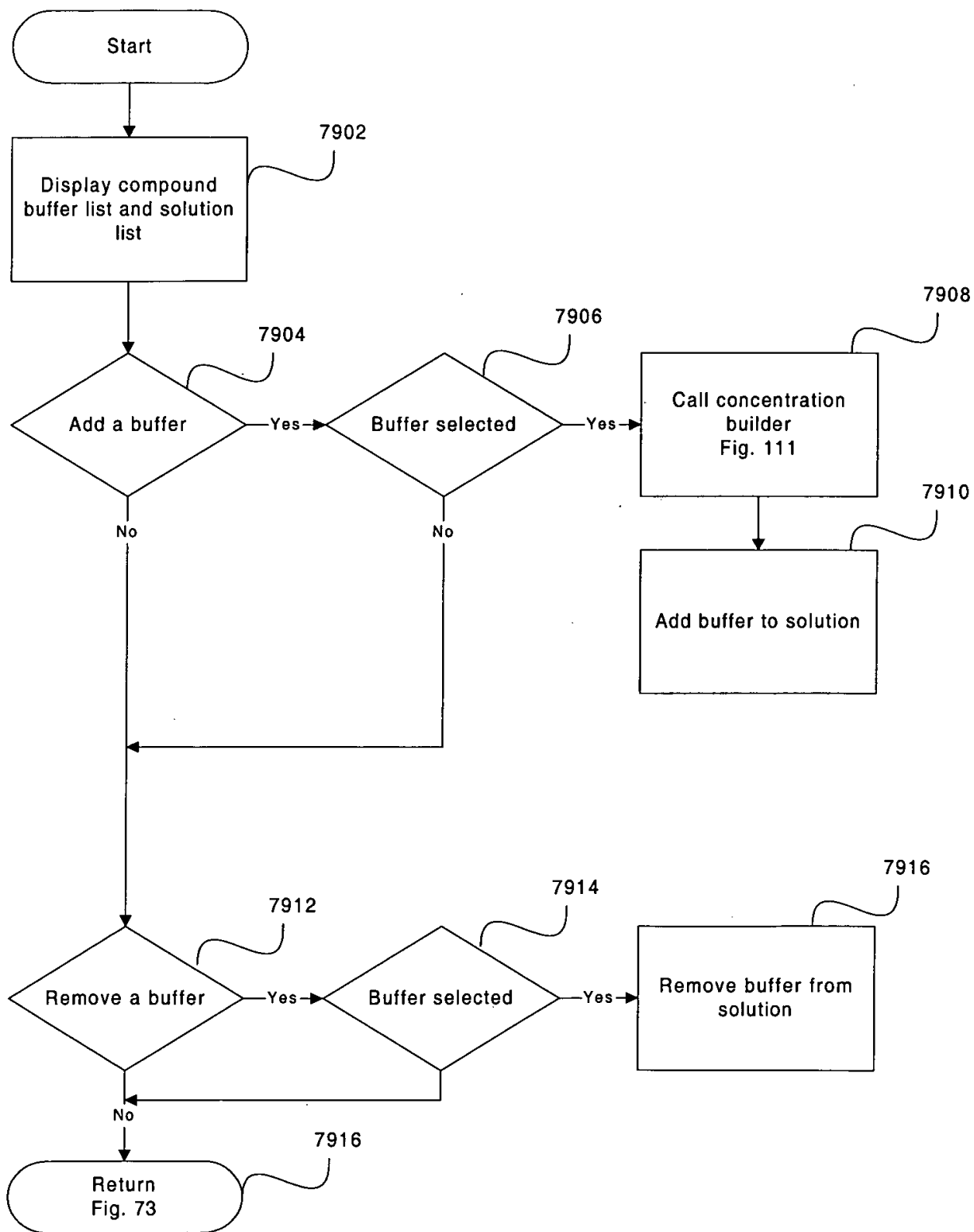


FIGURE 79

Formulation: ammsulf040400

Category: **Salt**

New Chemical

Chemical Name	Formul
ammonium chloride (NH4 chloride)	NH4Cl
ammonium dihydrogen phosphate (NH4 H2 phosph...	NH4H <sub>2</sub> P
ammonium formate (NH3 formate)	CH2O <sub>2</sub>
ammonium nitrate (NH4 nitrate)	NH4NO <sub>3</sub>
ammonium phosphate dibasic ((NH4)2 H phosph...	(NH4) <sub>2</sub> P
ammonium sulfate ((NH4)2 sulfate)	(NH4) <sub>2</sub> S
ammonium sulfate ((NH4)2 sulfate)	(NH4) <sub>2</sub> S
ammonium sulfate ((NH4)2 sulfate)	(NH4) <sub>2</sub> S

Solution Composition List:

Concentration	Chemical Name
200.000 mM	ammonium sulfate ((NH4)2 sulfate)

Delete Component

< Back Finish Cancel Help

8000 8004 8002 8006 8003 8001 8008 8010 8012 8014

Fig. 80



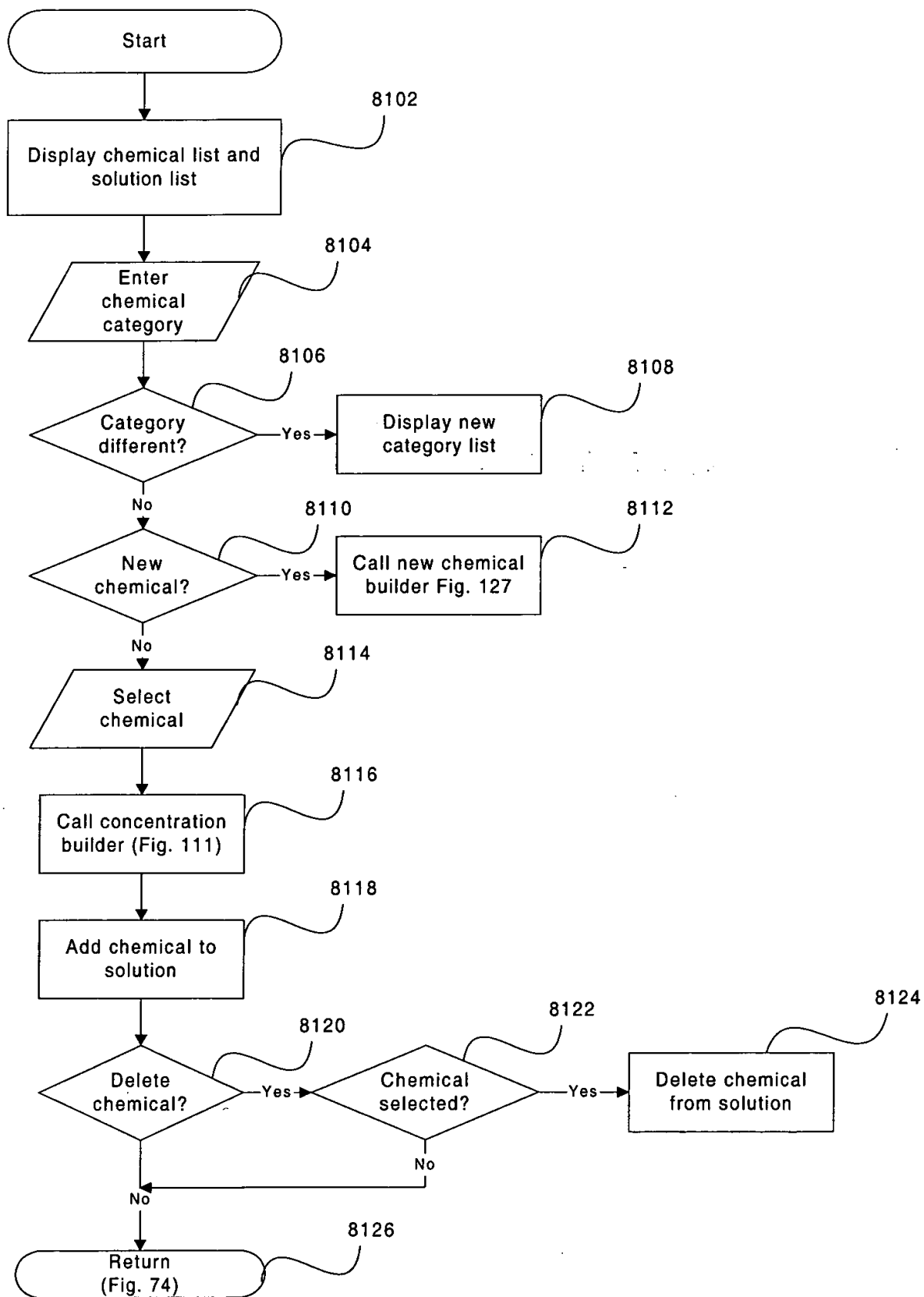


FIGURE 81

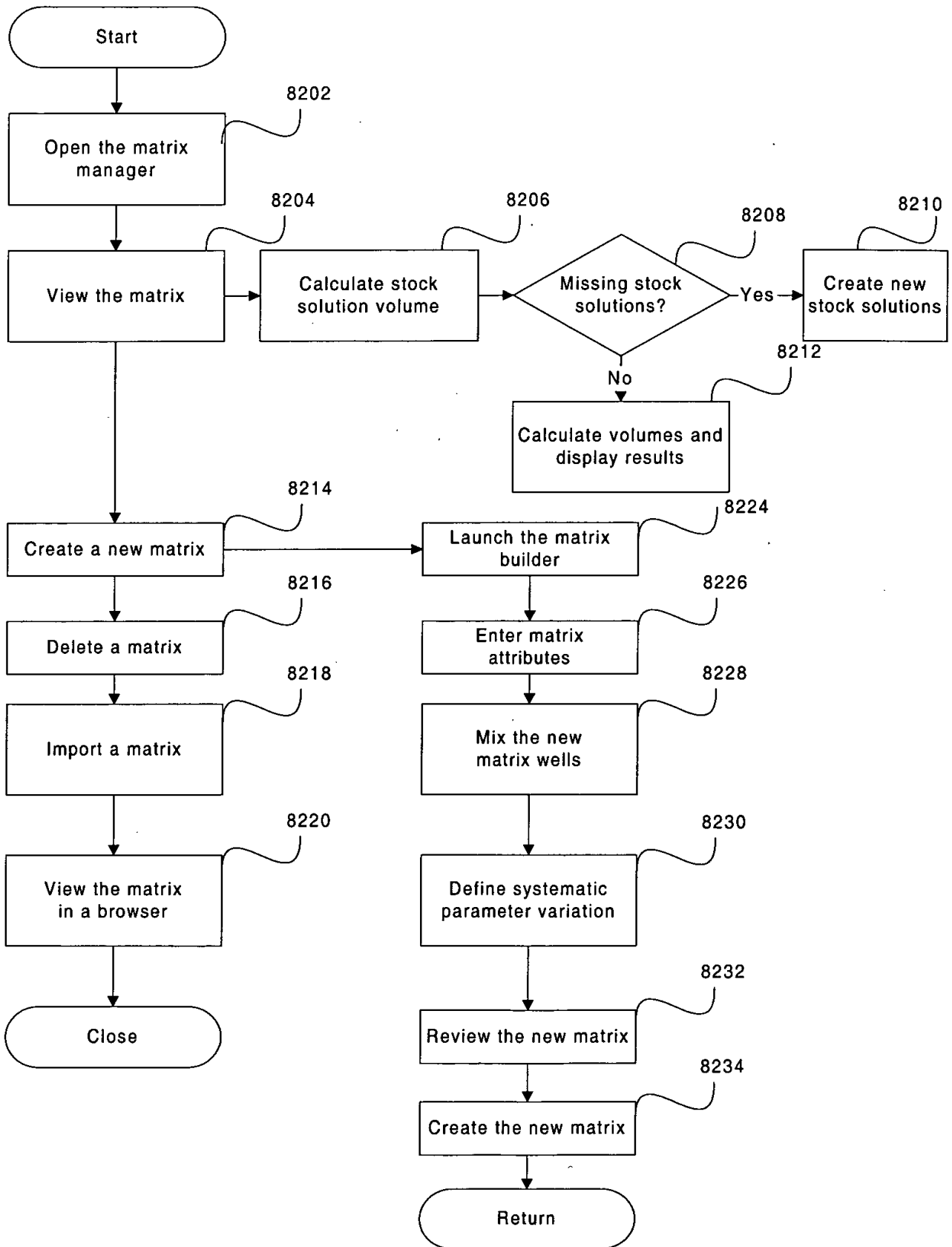


FIGURE 82

0963185-030200

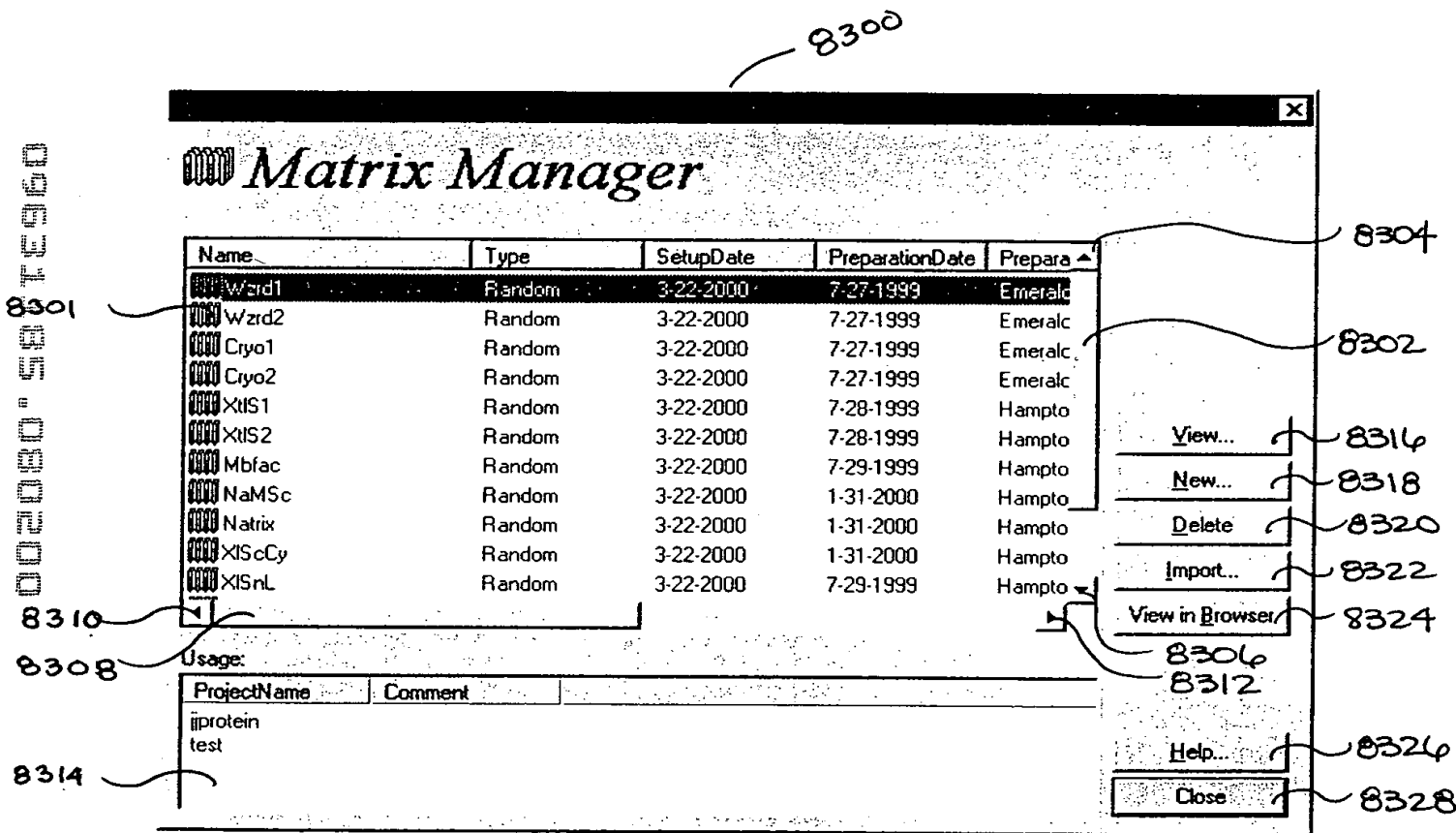


Fig. 83

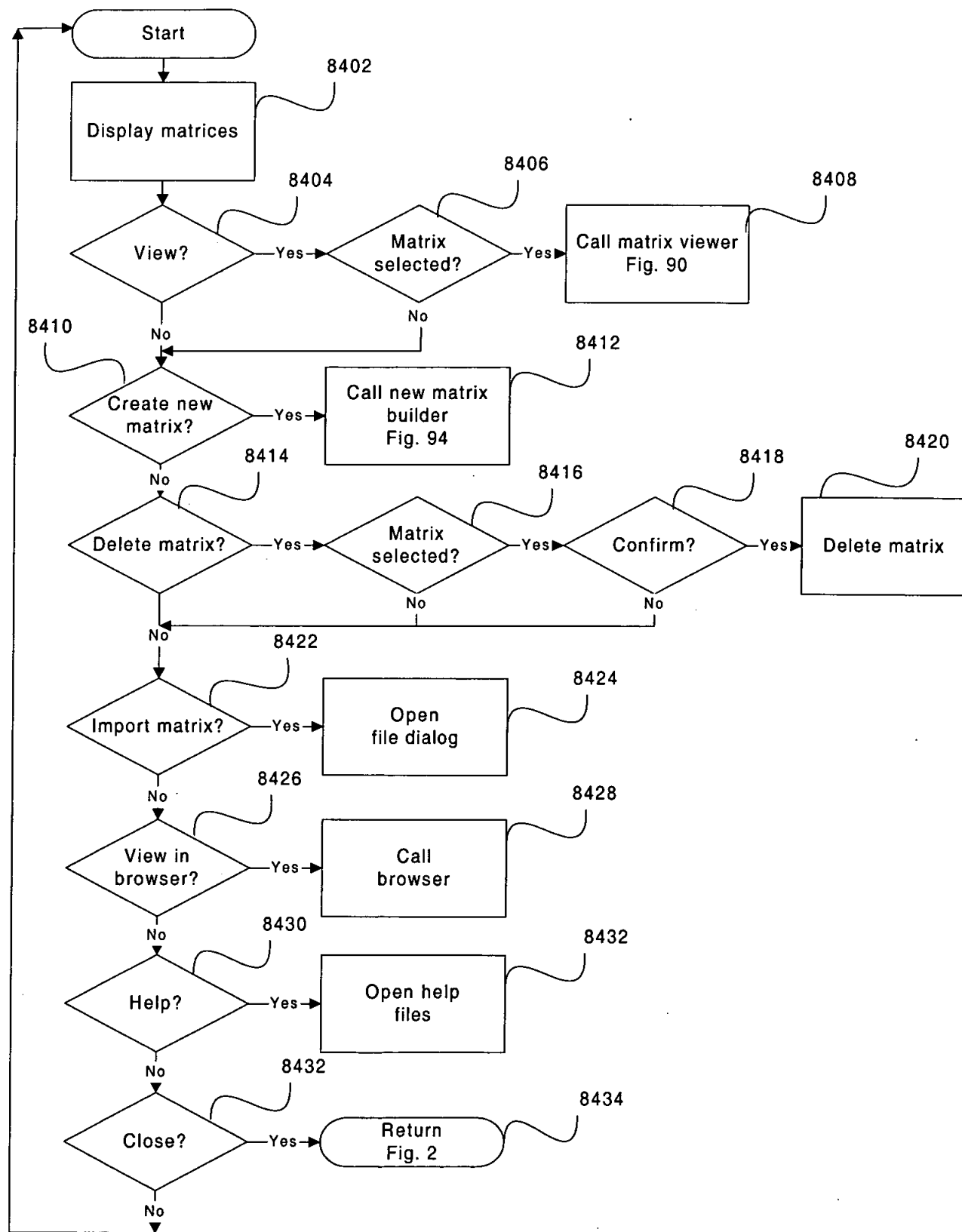


FIGURE 84

002080"587E960

8500

## Matrix Viewer

(2)	(2)	(2)	(2)	(2)	(2)
(2)	(2)	(2)	(2)	(2)	(2)
(2)	(2)	(2)	(2)	(2)	(2)
(2)	(2)	(2)	(2)	(2)	(2)

Matrix Name:  
newsys061599

Matrix Type:  
Systematic

Commercial:  
No

Preparator:  
Admin

X-Axis (systematically varied):  
polyethylene glycol 200

Y-Axis (systematically varied):  
sodium chloride

Comment:

Calc. Stock Sol. Vol. needed

OK

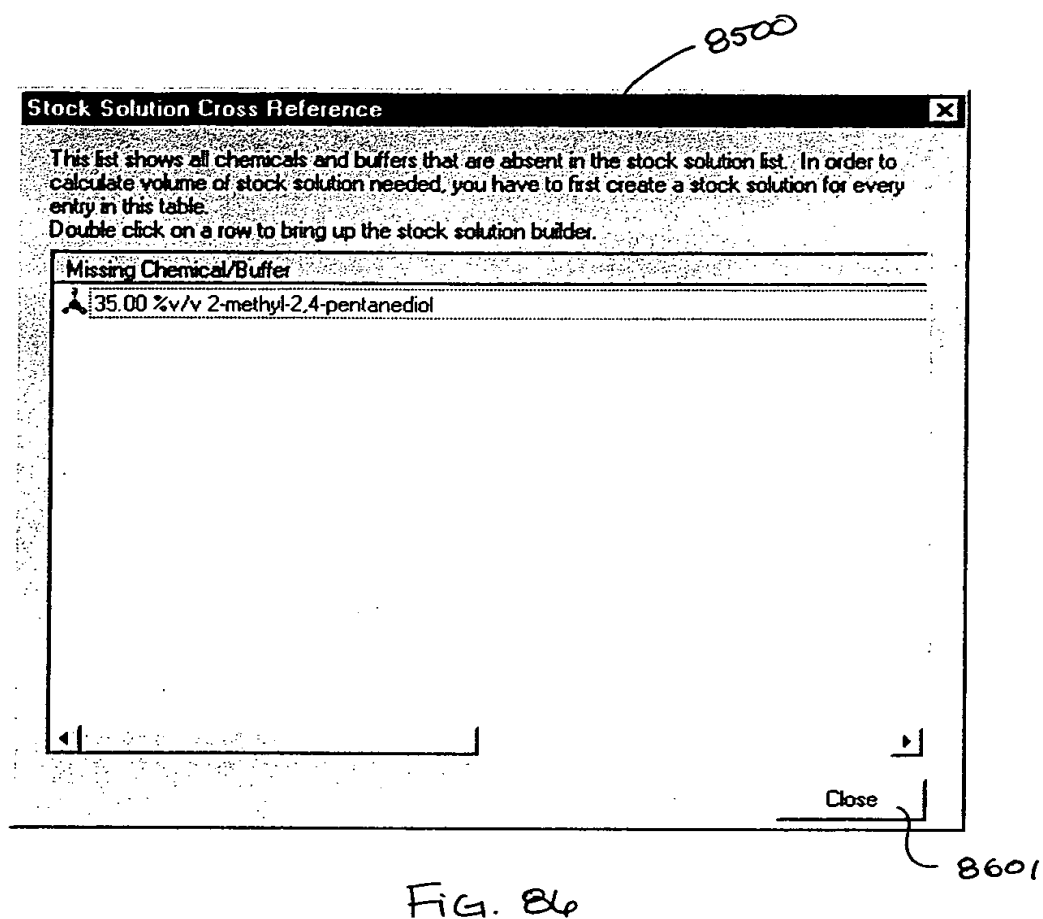
Cancel

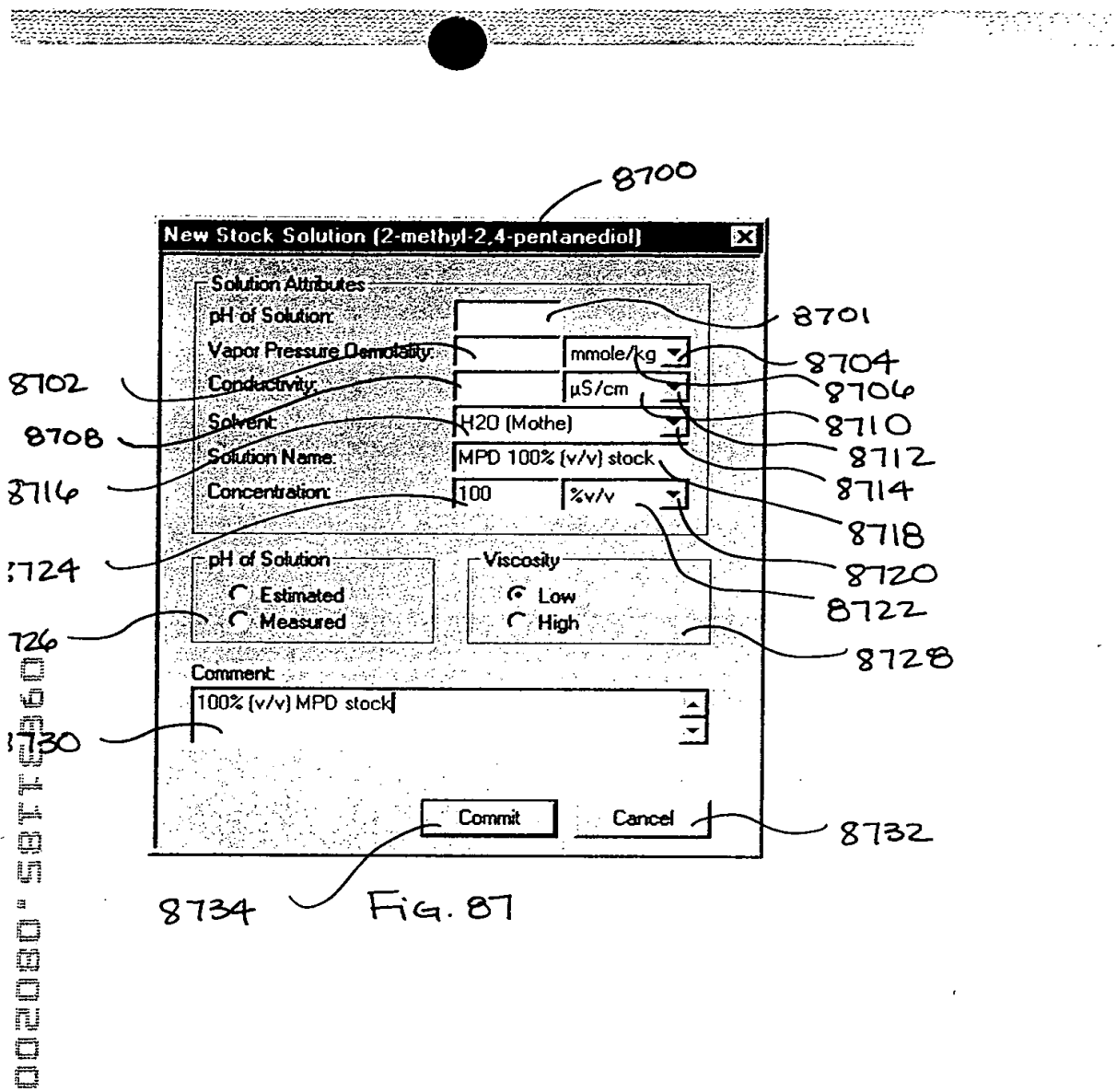
8502

8504

8506

Fig. 85





Stock solution volumes to build matrix newsys061599

What is the final desired Crystallant volume?

WellID	Volume	Stock Name	Stock Conc.	Chemical Name
1	1.000 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical ...)
1	0.200 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Ch...)
1	8.800 ml		n/a	H2O
2	1.500 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical ...)
2	0.200 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Ch...)
2	8.300 ml		n/a	H2O
3	2.000 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical ...)
3	0.200 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Ch...)
3	7.800 ml		n/a	H2O
4	2.500 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical ...)
4	0.200 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Ch...)
4	7.300 ml		n/a	H2O
5	3.000 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical ...)
5	0.200 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Ch...)

Close Help... View in Browser... Save to HTML...

Fig. 88

WellID	Volume	Stock Name	Stock Conc.	Chemical Name	Chemical Type	Final Conc.
1	1.000 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical Co.)	Precipitant	10.000 %v/v
1	0.200 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Chemical Co.)	Precipitant	100.000 mM

Fig. 89A



1	8.800 ml		n/a	H2O	Solvent	n/a
2	1.500 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical Co.)	Precipitant	15.000 %v/v
2	0.200 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Chemical Co.)	Precipitant	100.000 mM
2	8.300 ml		n/a	H2O	Solvent	n/a
3	2.000 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical Co.)	Precipitant	20.000 %v/v
3	0.200 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Chemical Co.)	Precipitant	100.000 mM
3	7.800 ml		n/a	H2O	Solvent	n/a
4	2.500 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical Co.)	Precipitant	25.000 %v/v
4	0.200 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Chemical Co.)	Precipitant	100.000 mM
4	7.300 ml		n/a	H2O	Solvent	n/a
5	3.000 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical Co.)	Precipitant	30.000 %v/v
5	0.200 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Chemical Co.)	Precipitant	100.000 mM
5	6.800 ml		n/a	H2O	Solvent	n/a
6	3.500 ml	PEG-200	100.000	PEG-200	Precipitant	35.000

Fig. 89B

		stock	%v/v	(Sigma Chemical Co.)	t	%v/v
6	0.200 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Chemical Co.)	Precipitant	100.000 mM
6	6.300 ml		n/a	H <sub>2</sub> O	Solvent	n/a
7	1.000 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical Co.)	Precipitant	10.000 %v/v
7	0.400 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Chemical Co.)	Precipitant	200.000 mM
7	8.600 ml		n/a	H <sub>2</sub> O	Solvent	n/a
8	1.500 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical Co.)	Precipitant	15.000 %v/v
8	0.400 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Chemical Co.)	Precipitant	200.000 mM
8	8.100 ml		n/a	H <sub>2</sub> O	Solvent	n/a
9	2.000 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical Co.)	Precipitant	20.000 %v/v
9	0.400 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Chemical Co.)	Precipitant	200.000 mM
9	7.600 ml		n/a	H <sub>2</sub> O	Solvent	n/a
10	2.500 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical Co.)	Precipitant	25.000 %v/v

Fig. 89C

				Co.)		
10	0.400 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Chemical Co.)	Precipitant	200.000 mM
10	7.100 ml		n/a	H <sub>2</sub> O	Solvent	n/a
11	3.000 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical Co.)	Precipitant	30.000 %v/v
11	0.400 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Chemical Co.)	Precipitant	200.000 mM
11	6.600 ml		n/a	H <sub>2</sub> O	Solvent	n/a
12	3.500 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical Co.)	Precipitant	35.000 %v/v
12	0.400 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Chemical Co.)	Precipitant	200.000 mM
12	6.100 ml		n/a	H <sub>2</sub> O	Solvent	n/a
13	1.000 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical Co.)	Precipitant	10.000 %v/v
13	0.600 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Chemical Co.)	Precipitant	300.000 mM
13	8.400 ml		n/a	H <sub>2</sub> O	Solvent	n/a
14	1.500 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical Co.)	Precipitant	15.000 %v/v
14	0.600 ml	sodium	5000.000	sodium	Precipitant	300.000

Fig. 80D

		chloride 5 M stock	mM	chloride (Sigma Chemical Co.)	t	mM
14	7.900 ml		n/a	H <sub>2</sub> O	Solvent	n/a
15	2.000 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical Co.)	Precipitan t	20.000 %v/v
15	0.600 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Chemical Co.)	Precipitan t	300.000 mM
15	7.400 ml		n/a	H <sub>2</sub> O	Solvent	n/a
16	2.500 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical Co.)	Precipitan t	25.000 %v/v
16	0.600 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Chemical Co.)	Precipitan t	300.000 mM
16	6.900 ml		n/a	H <sub>2</sub> O	Solvent	n/a
17	3.000 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical Co.)	Precipitan t	30.000 %v/v
17	0.600 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Chemical Co.)	Precipitan t	300.000 mM
17	6.400 ml		n/a	H <sub>2</sub> O	Solvent	n/a
18	3.500 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical Co.)	Precipitan t	35.000 %v/v
18	0.600 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma	Precipitan t	300.000 mM

Fig. 80E

				Chemical Co.)		
18	5.900 ml		n/a	H2O	Solvent	n/a
19	1.000 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical Co.)	Precipitant	10.000 %v/v
19	0.800 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Chemical Co.)	Precipitant	400.000 mM
19	8.200 ml		n/a	H2O	Solvent	n/a
20	1.500 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical Co.)	Precipitant	15.000 %v/v
20	0.800 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Chemical Co.)	Precipitant	400.000 mM
20	7.700 ml		n/a	H2O	Solvent	n/a
21	2.000 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical Co.)	Precipitant	20.000 %v/v
21	0.800 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Chemical Co.)	Precipitant	400.000 mM
21	7.200 ml		n/a	H2O	Solvent	n/a
22	2.500 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical Co.)	Precipitant	25.000 %v/v
22	0.800 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Chemical Co.)	Precipitant	400.000 mM

Fig. 80F

22	6.700 ml		n/a	H2O	Solvent	n/a
23	3.000 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical Co.)	Precipitant	30.000 %v/v
23	0.800 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Chemical Co.)	Precipitant	400.000 mM
23	6.200 ml		n/a	H2O	Solvent	n/a
24	3.500 ml	PEG-200 stock	100.000 %v/v	PEG-200 (Sigma Chemical Co.)	Precipitant	35.000 %v/v
24	0.800 ml	sodium chloride 5 M stock	5000.000 mM	sodium chloride (Sigma Chemical Co.)	Precipitant	400.000 mM
24	5.700 ml		n/a	H2O	Solvent	n/a

Fig. 89G

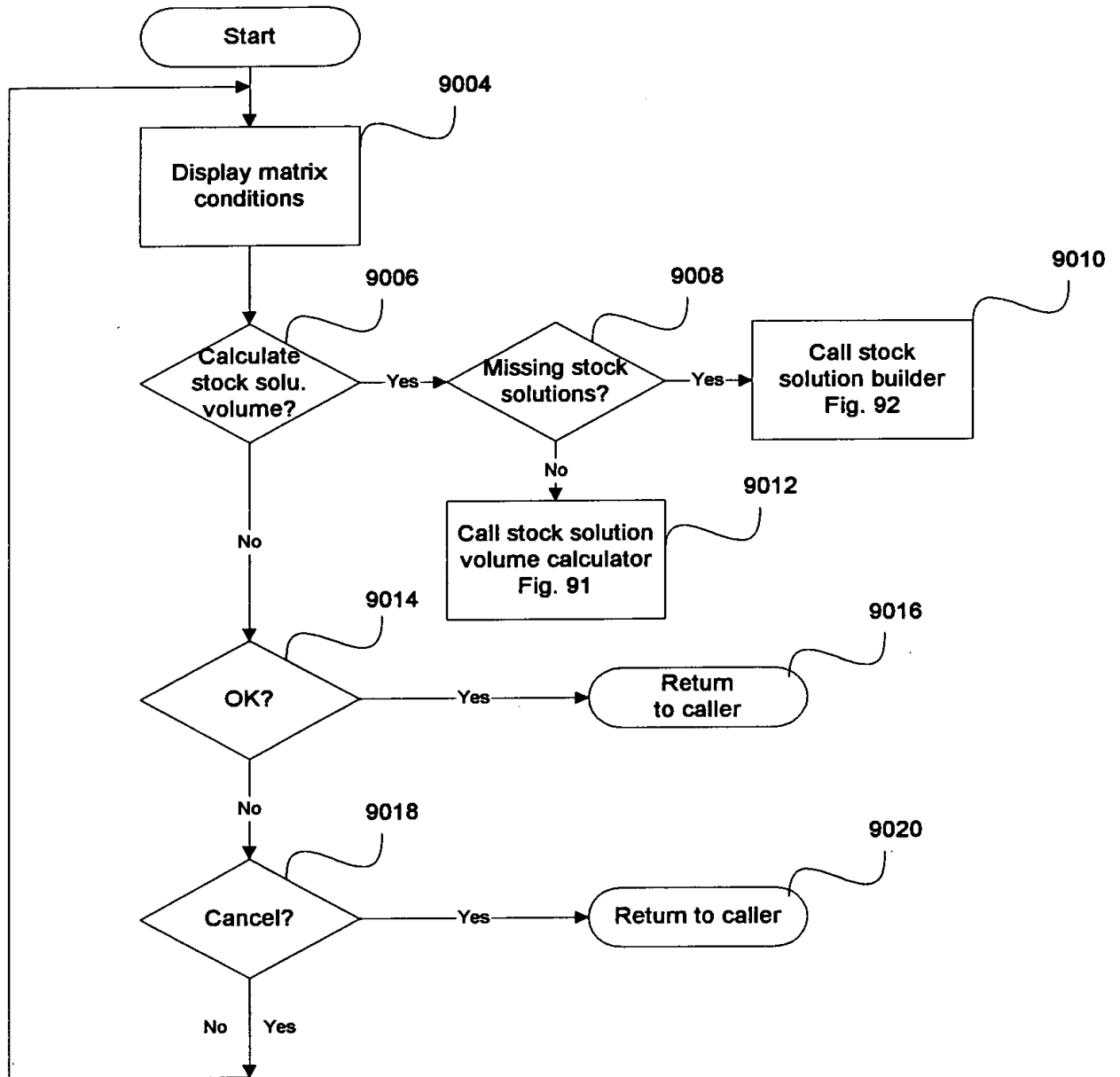


FIGURE 90

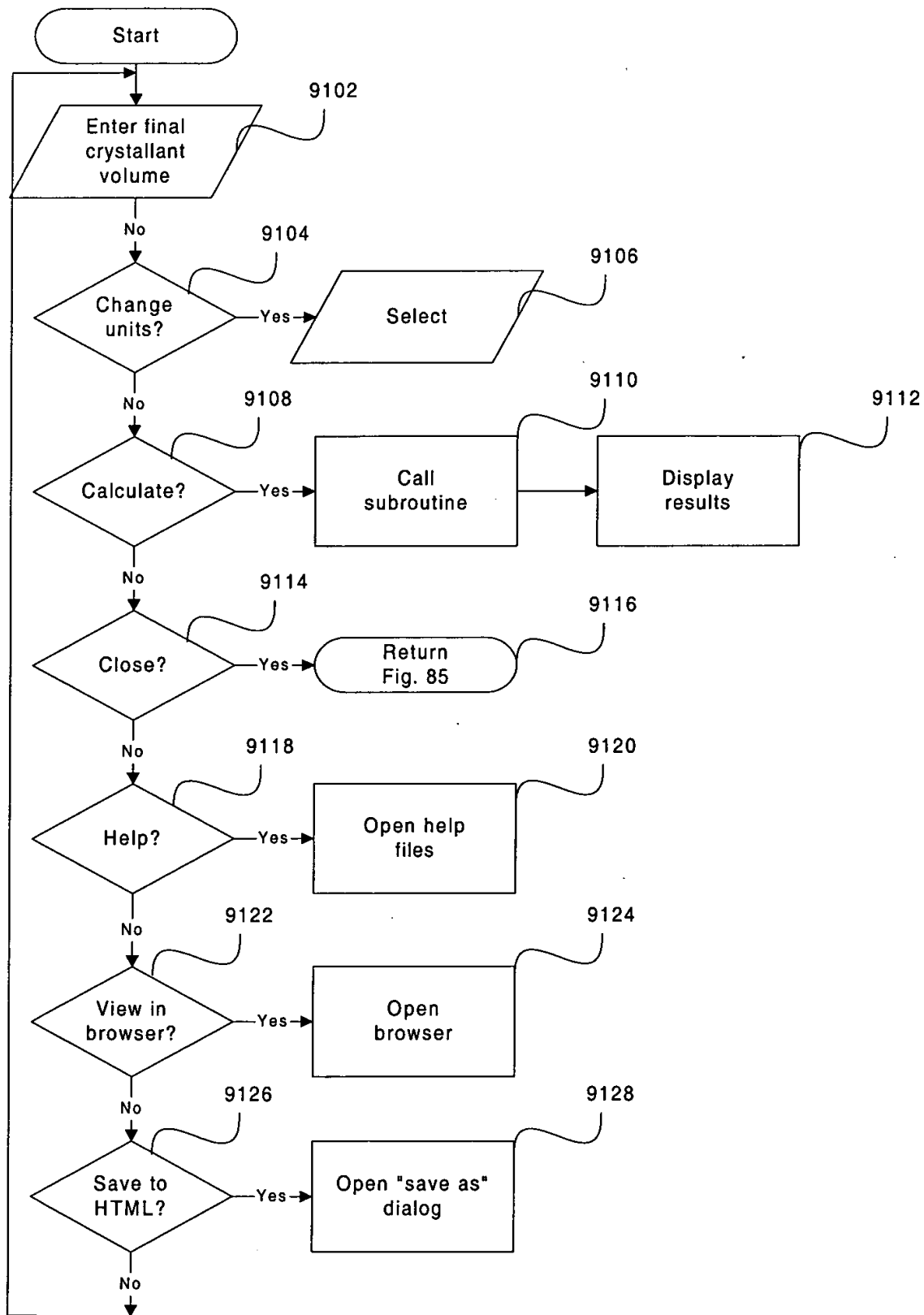


FIGURE 91



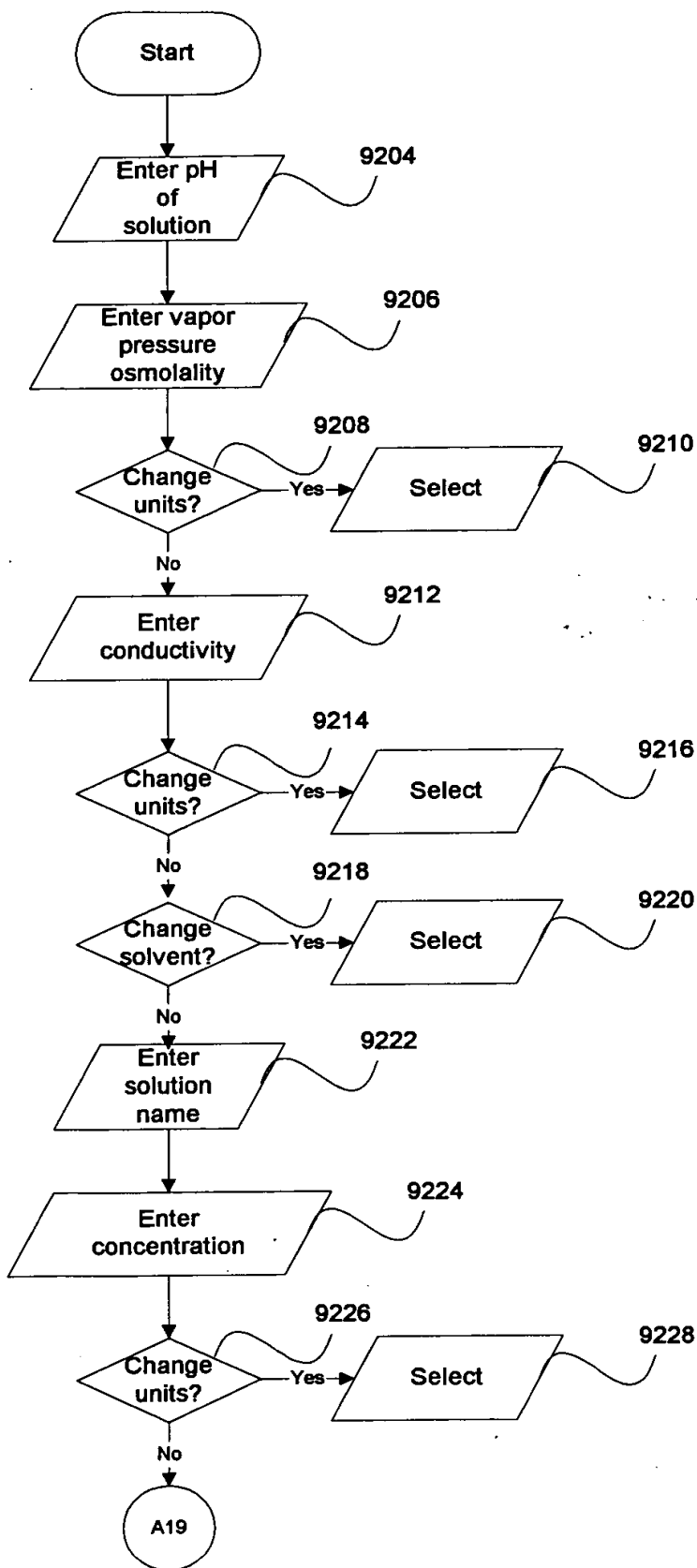


FIGURE 92

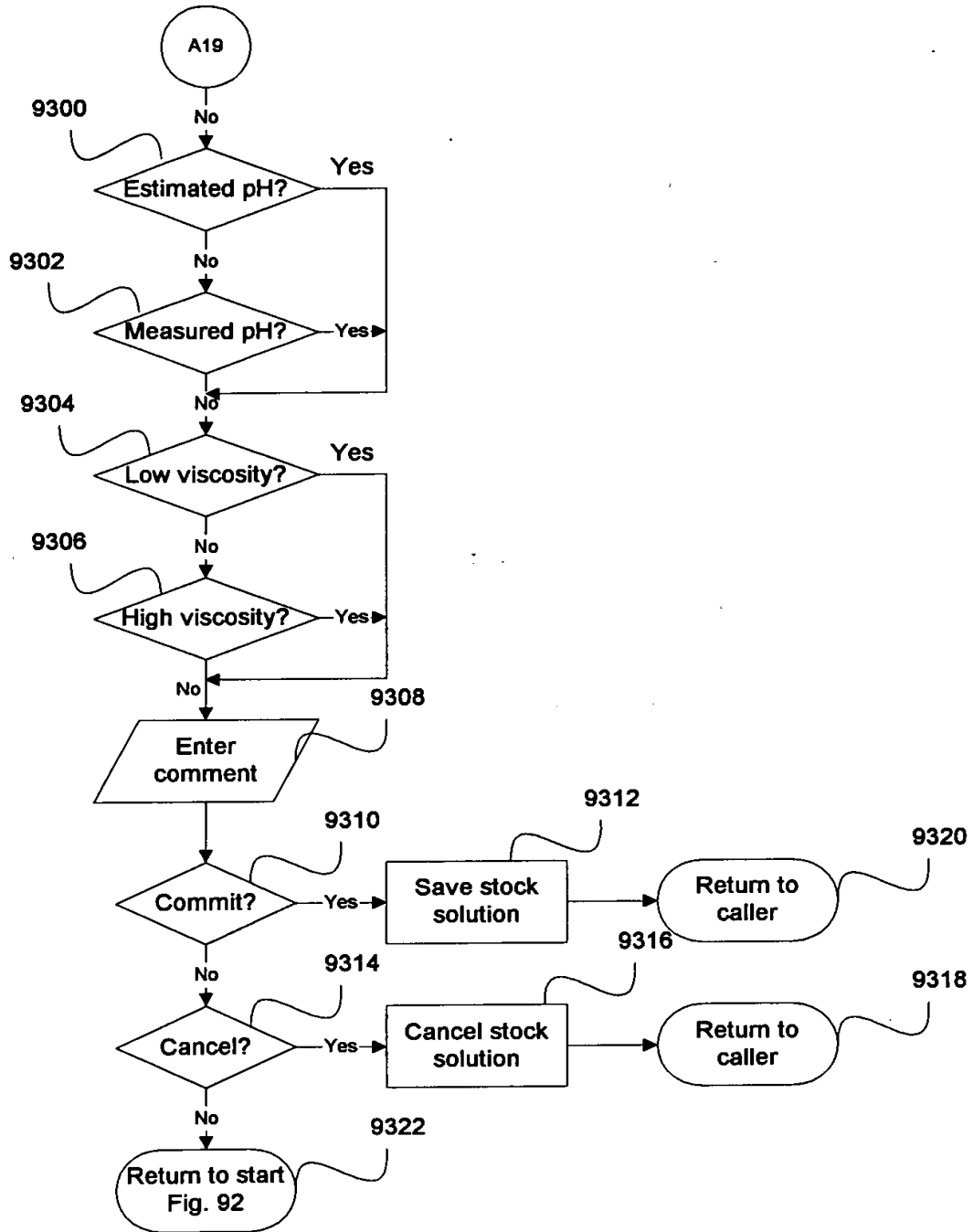


FIGURE 93

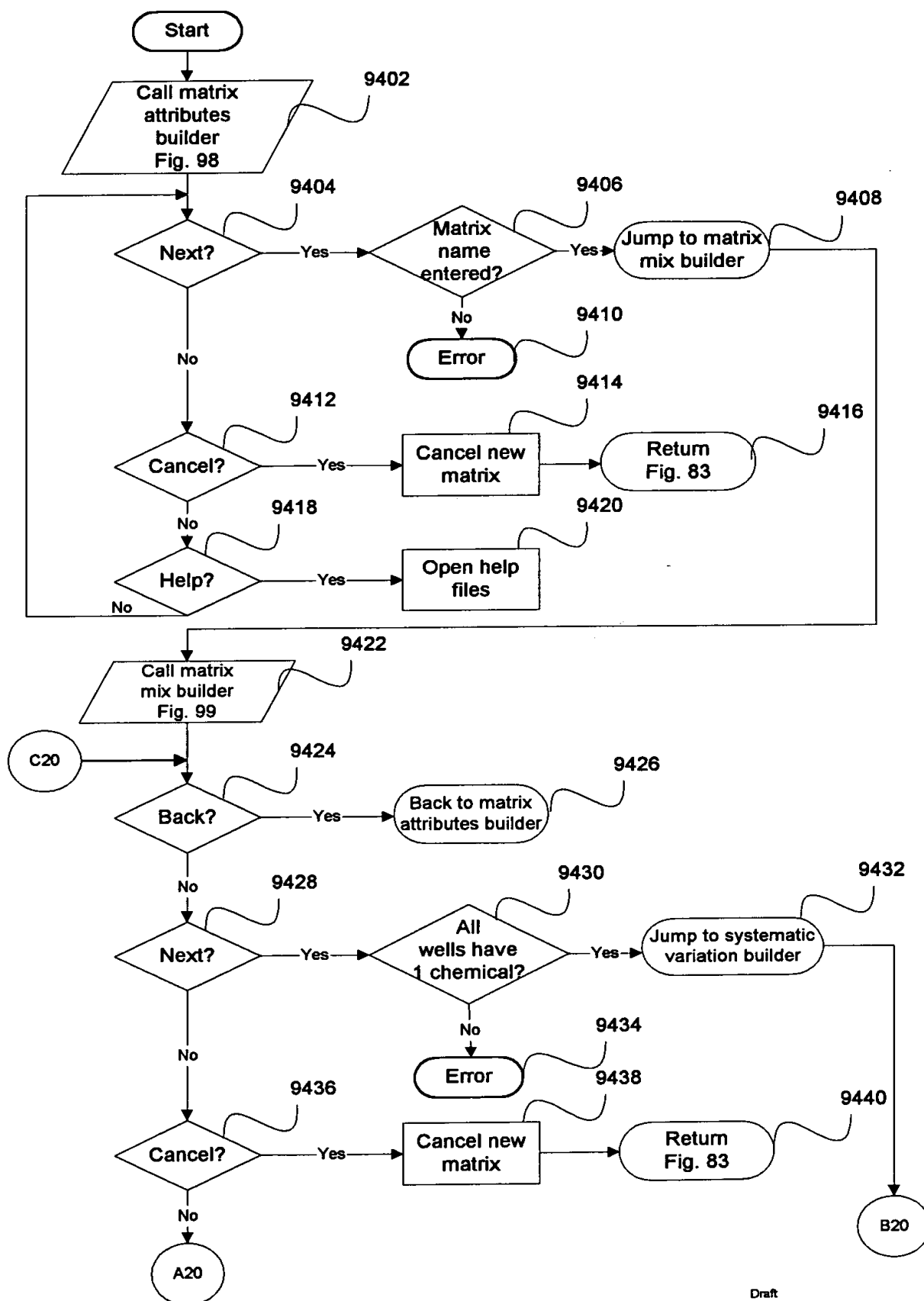


FIGURE 94

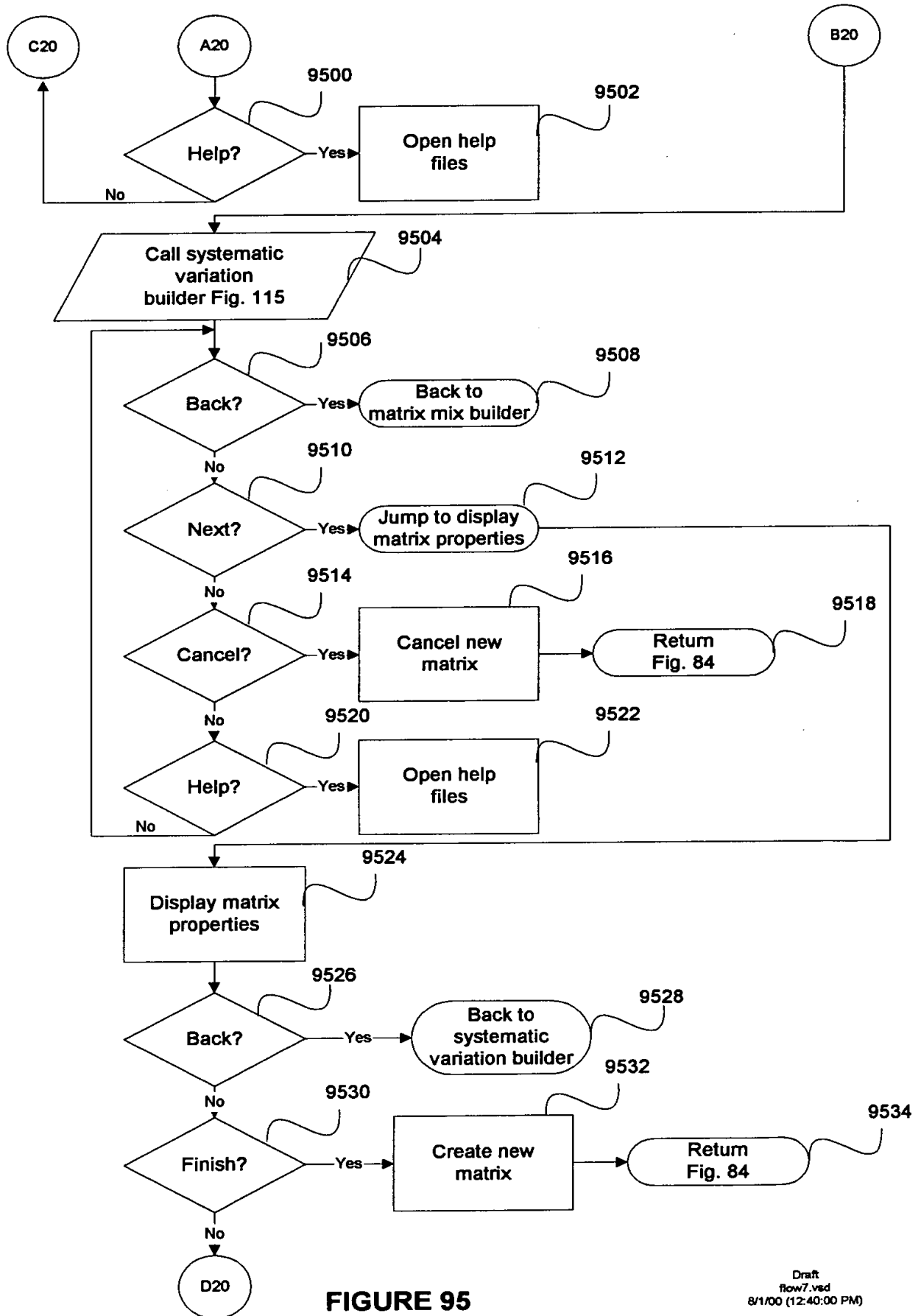


FIGURE 95

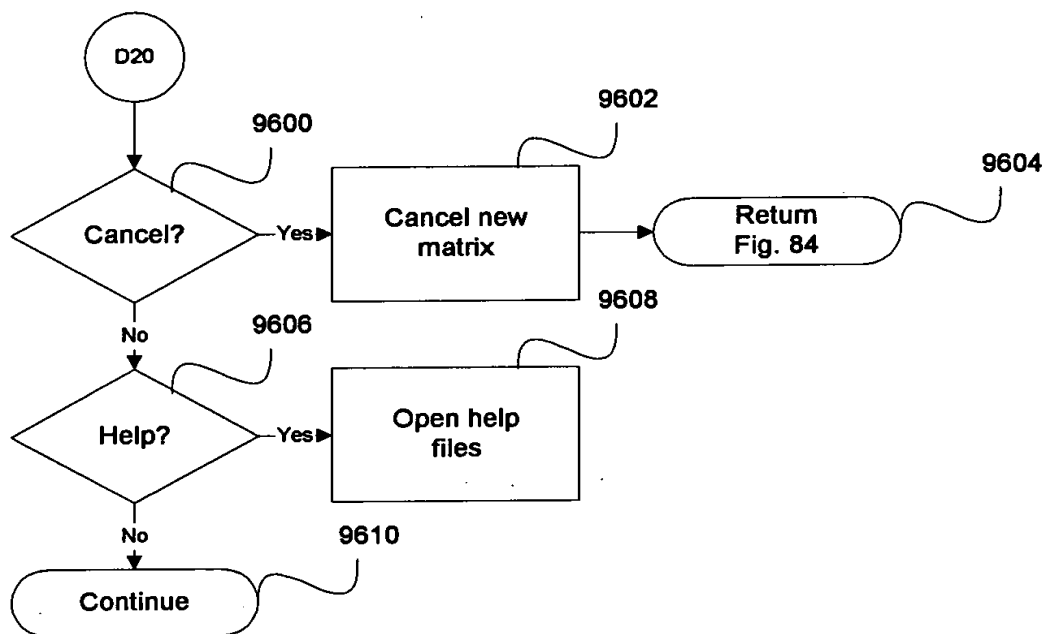


FIGURE 96

The screenshot shows a window titled "Matrix Wizard" with a close button (X) in the top right corner. On the left side of the window is a grayscale image of a matrix, which appears to be a grid of small, dark, circular elements. The right side of the window contains several input fields and a checkbox. The "Matrix Name" field contains the text "new48040400". The "Well Count" field is a spinner box showing the value "48". The "Column Count" field is a spinner box showing the value "6". Below these fields is a checkbox labeled "Commercial. (Matrix is available from a commercial source)". Below the checkbox is a "Preparator" field containing the text "Admin". At the bottom of the window are four buttons: "< Back", "Next >", "Cancel", and "Help". Handwritten reference numerals are placed around the window: 9700 points to the title bar; 9704, 9706 point to the Matrix Name field; 9701 points to the Well Count field; 9702 points to the Column Count field; 9708 points to the Commercial checkbox; 9710, 9712 point to the Preparator field; 9714 points to the Commercial checkbox label; 9718 points to the Preparator field; 9716 points to the dropdown arrow of the Preparator field; 9720 points to the "< Back" button; 9722 points to the "Next >" button; 9724 points to the "Cancel" button; and 9726 points to the "Help" button.

Matrix Wizard

Matrix Name: new48040400

Well Count: 48

Column Count: 6

Commercial. (Matrix is available from a commercial source)

Preparator: Admin

< Back Next > Cancel Help

Fig. 97

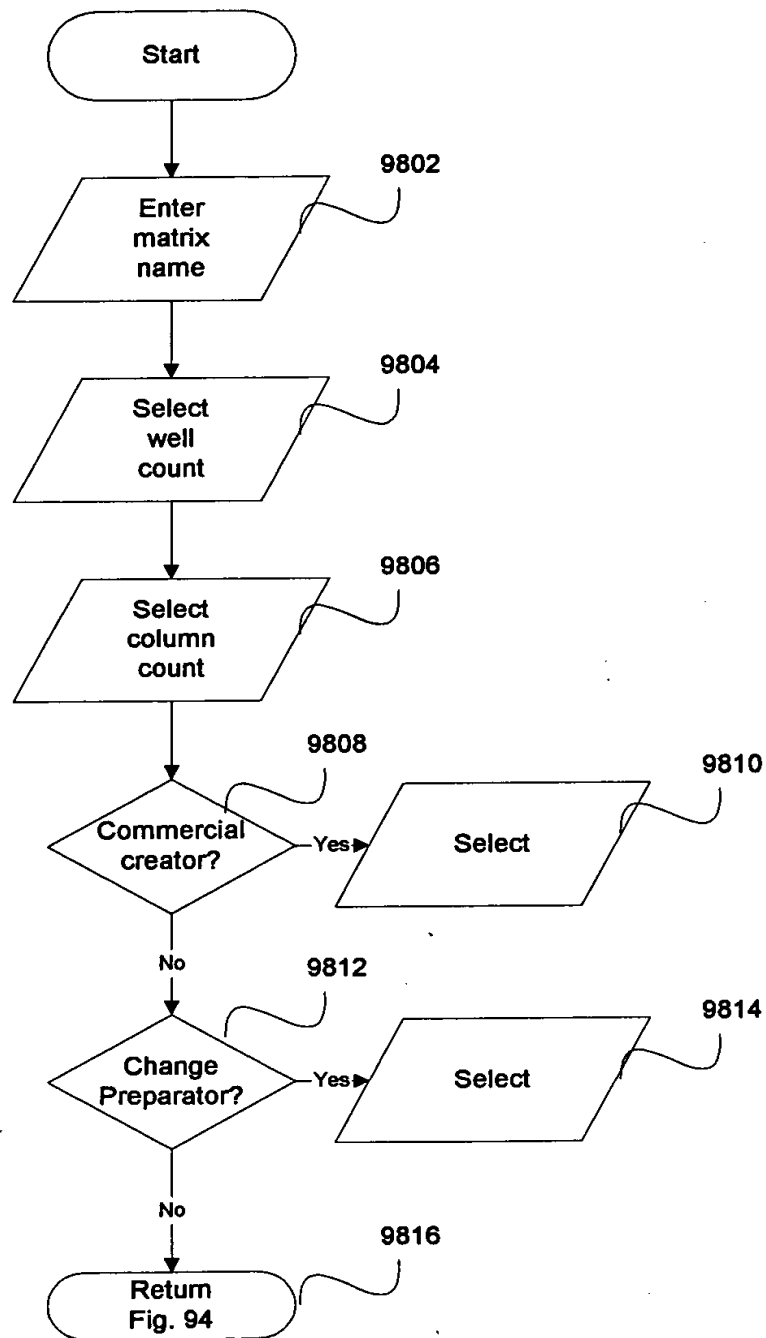


FIGURE 98

```

graph TD
    Start([Start]) --> 9902[/Select source matrix/]
    9902 --> 9904[Display source matrix wells]
    9904 --> 9906{Select all wells?}
    9906 -- Yes --> 9908[Toggle select all/ unselect all]
    9906 -- No --> 9910{Copy all?}
    9910 -- Yes --> 9912[Copy all source matrix wells to new matrix wells]
    9910 -- No --> 9914[/Select well/]
    9914 --> 9916[/Select a source matrix well/]
    9916 --> 9918{Copy?}
    9918 -- Yes --> 9920{Well selected?}
    9920 -- Yes --> 9922[Copy source matrix well to selected new matrix well]
    9920 -- No --> 9924{Delete component?}
    9918 -- No --> 9924
    9924 -- Yes --> 9926{Well selected?}
    9926 -- Yes --> 9928[Call well crystallant composition builder Fig. 107]
    9926 -- No --> 9930{Well properties?}
    9924 -- No --> 9930
    9930 -- Yes --> 9932{Well selected?}
    9932 -- Yes --> 9934[Call solution properties builder Fig. 108]
    9932 -- No --> A21((A21))
    9930 -- No --> A21
  
```

Draft  
flow7.vsd  
8/1/00 (12:41:58 PM)



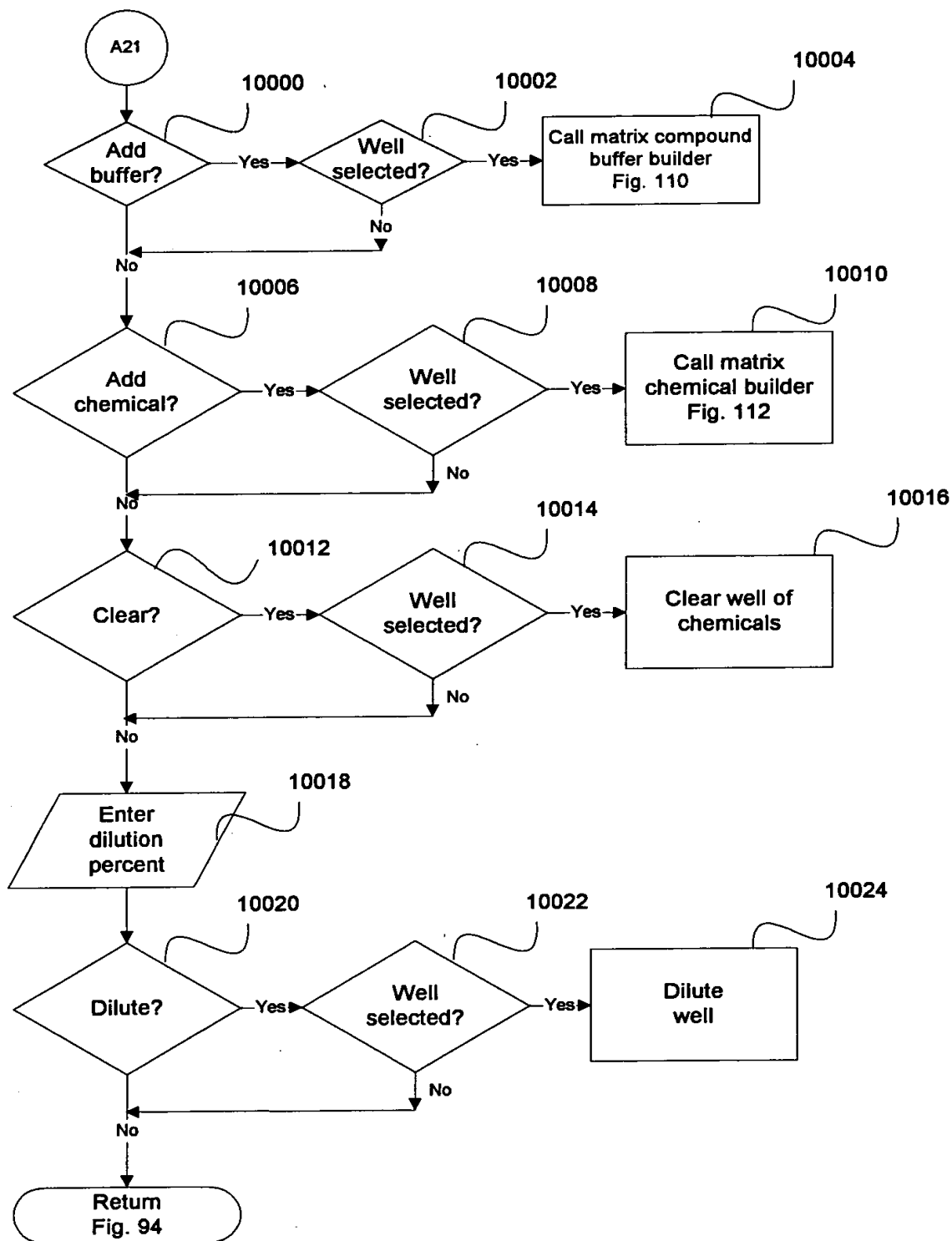


FIGURE 100

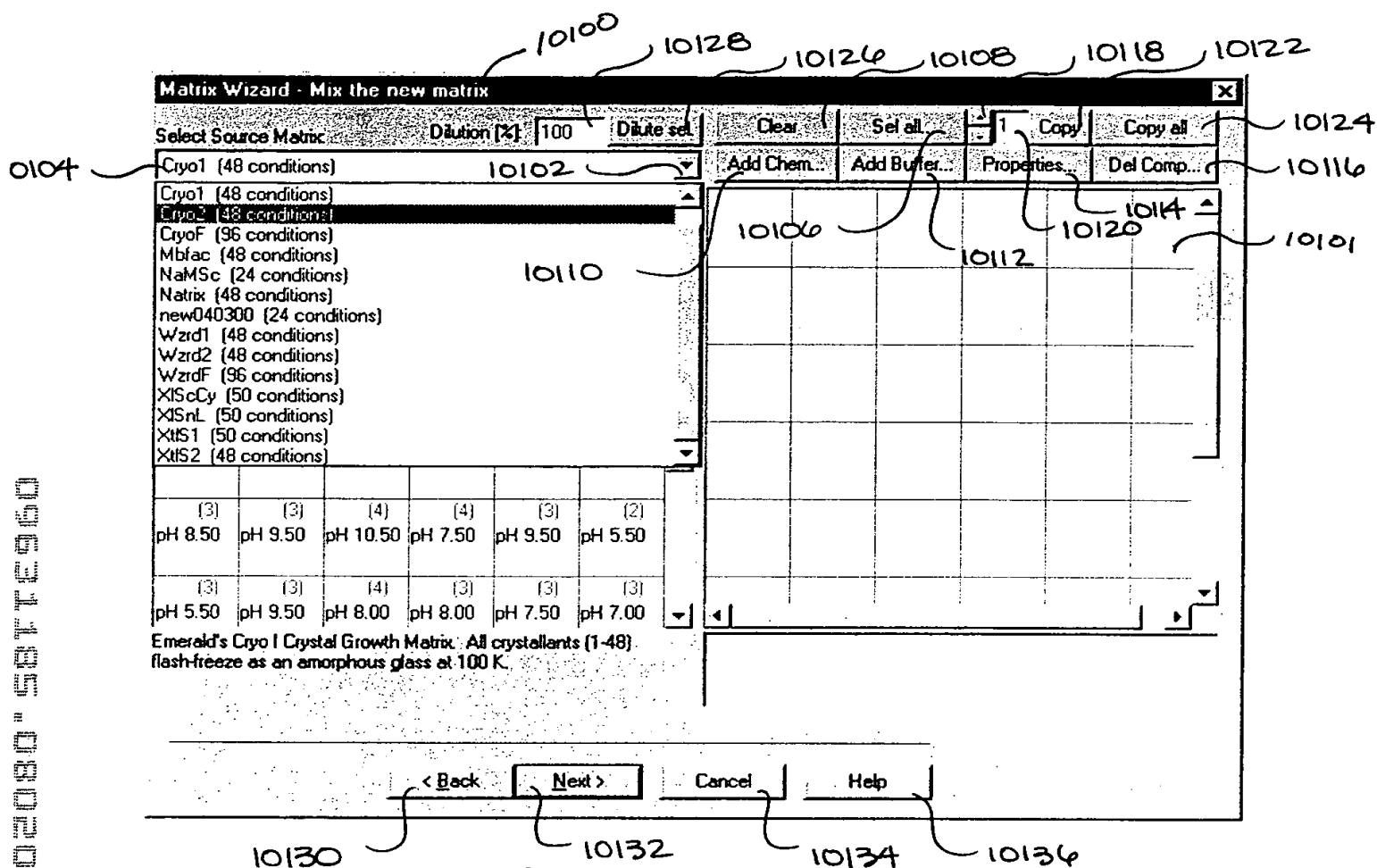


FIG. 101

Matrix Wizard - Mix the new matrix

Select Source Matrix: **Dilution [%]:** 50 **Dilute sel:** **Clear** **Set all** **Copy** **Copy all**

**Cryo1 (48 conditions)** **Add Chem...** **Add Buffer...** **Properties...** **Del Comp...**

(2) pH 4.20	(2) pH 4.50	(2) pH 5.50	(3) pH 7.50	(3) pH 5.50	(3) pH 6.50	(2) pH 4.20	(2) pH 4.20	(2) pH 4.20	(2) pH 4.20
(3) pH 8.50	(2) pH 6.50	(2) pH 4.20	(2) pH 8.00	(3) pH 8.50	(3) pH 4.50	<p>- Well 1 -</p> <p>Compound Buffers: 50.000 mM (Na2 H phosphate, citric acid) pH 4.20</p> <p>Chemicals: 20.000 %v/v MPD, Precipitant (Fluka Chemical Corp. 68340)</p> <p>Solution Properties: Final pH: 4.20 est. Conductivity: n/a Vapor Pressure Osmolality: n/a Viscosity: Low Solvent: H2O</p>			
(3) pH 6.00	(4) pH 4.20	(3) pH 9.50	(4) pH 6.00	(2) pH 7.50	(3) pH 8.00				
(2) pH 8.50	(3) pH 5.50	(3) pH 4.50	(2) pH 6.20	(3) pH 7.00	(3) pH 6.20				
(3) pH 8.50	(3) pH 9.50	(4) pH 10.50	(4) pH 7.50	(3) pH 9.50	(2) pH 5.50				
(3) pH 5.50	(3) pH 9.50	(4) pH 8.00	(3) pH 8.00	(3) pH 7.50	(3) pH 7.00				

Emerald's Cryo I Crystal Growth Matrix. All crystallants (1-48) flash-freeze as an amorphous glass at 100 K.

< Back Next > Cancel Help

FIG. 102

10300

**Crystallant Composition - Removal List** X

Check the box for the Chemicals to remove from selected wells:

Chemical Name	Abbreviation	Formula
<input type="checkbox"/> 2-methyl-2,4-pentanediol	MPD	C6H14O2

◀ ▶

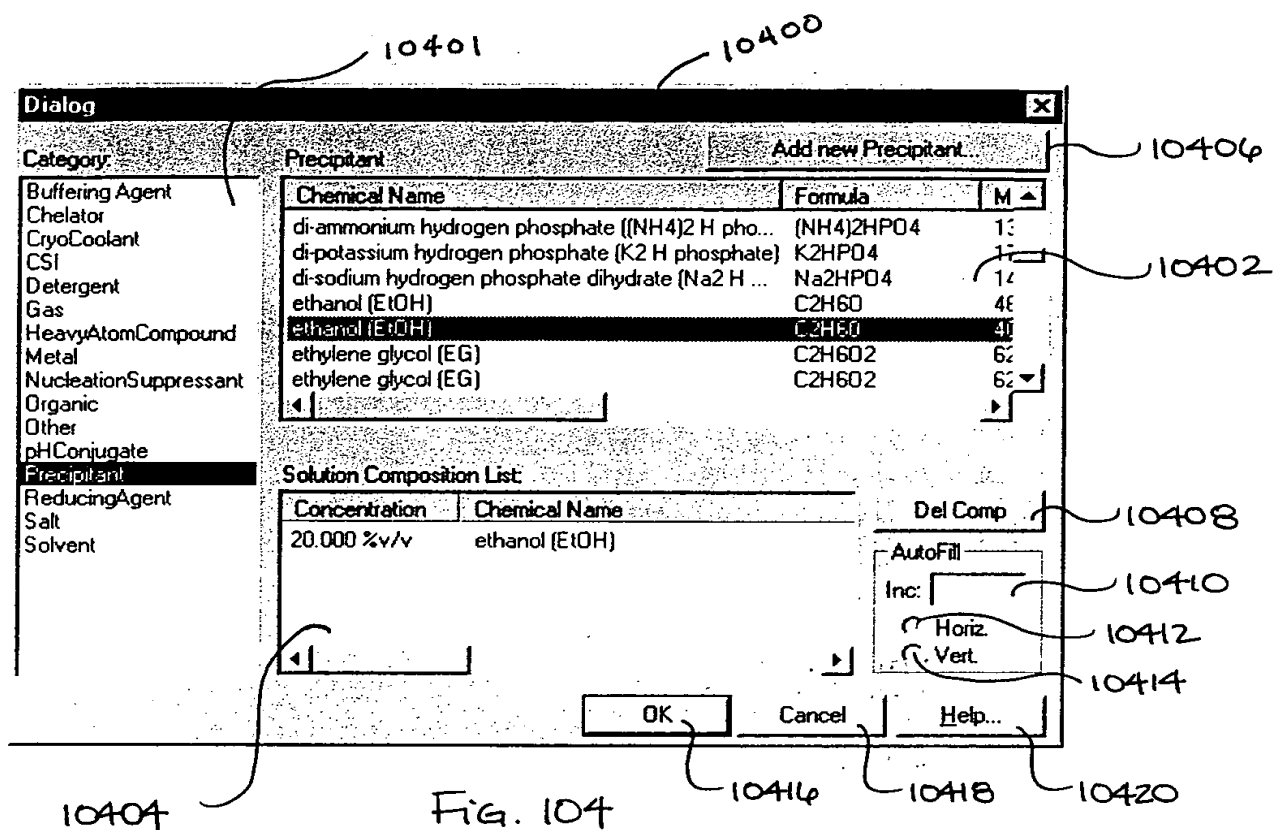
Check the box for the Compound Buffers to remove from selected wells:

Buffer PH	Buffering Agent	pH Conjugate
<input type="checkbox"/> 4.20	sodium phosphate dibasic (N...	citric acid monohydrate (citric...

◀ ▶

10304a      10301      10302      10308      10306

Fig. 103



**Dialog**

**Category:**

- Buffering Agent
- Chelator
- CryoCoolant
- CSI
- Detergent
- Gas
- HeavyAtomCompound
- Metal
- NucleationSuppressant
- Organic
- Other
- pHConjugate
- Precipitant**
- ReducingAgent
- Salt
- Solvent

**Precipitant**

Chemical Name	Formula	M
polyethylene glycol 12000 (PEG-12000)	H(OCH <sub>2</sub> CH <sub>2</sub> O) <sub>n</sub> H	12
polyethylene glycol 1500 (PEG-1500)	H(OCH <sub>2</sub> CH <sub>2</sub> O) <sub>n</sub> H	15
polyethylene glycol 1500 (PEG-1500)	H(OCH <sub>2</sub> CH <sub>2</sub> O) <sub>n</sub> H	15
polyethylene glycol 200 (PEG-200)	H(OCH <sub>2</sub> CH <sub>2</sub> O) <sub>n</sub> H	20
polyethylene glycol 200 (PEG-200)	H(OCH <sub>2</sub> CH <sub>2</sub> O) <sub>n</sub> H	20
polyethylene glycol 200 (PEG-200)	H(OCH <sub>2</sub> CH <sub>2</sub> O) <sub>n</sub> H	20
polyethylene glycol 2000 dimethyl ether (PEG-2000...)	H(OCH <sub>2</sub> CH <sub>2</sub> O) <sub>n</sub> H	20

**Add new Precipitant**

**Solution Composition List**

Concentration	Chemical Name
10.000 %v/v	polyethylene glycol 200 (PEG-200)

**Del Comp**

AutoFill

Inc: 5

☒ Horiz

☐ Vert

OK Cancel Help...

Fig. 105

09631185, 080200

10600

**Matrix Wizard - Mix the new matrix**

Select Source Matrix:  Dilute sel:

<Select Matrix>

(1)	(1)	(1)	(1)	(1)	(1)
(1)	(1)	(1)	(1)	(1)	(1)
(1)	(1)	(1)	(1)	(1)	(1)
(1)	(1)	(1)	(1)	(1)	(1)

< Back   Next >   Cancel   Help

Fig. 106

002030-587E960

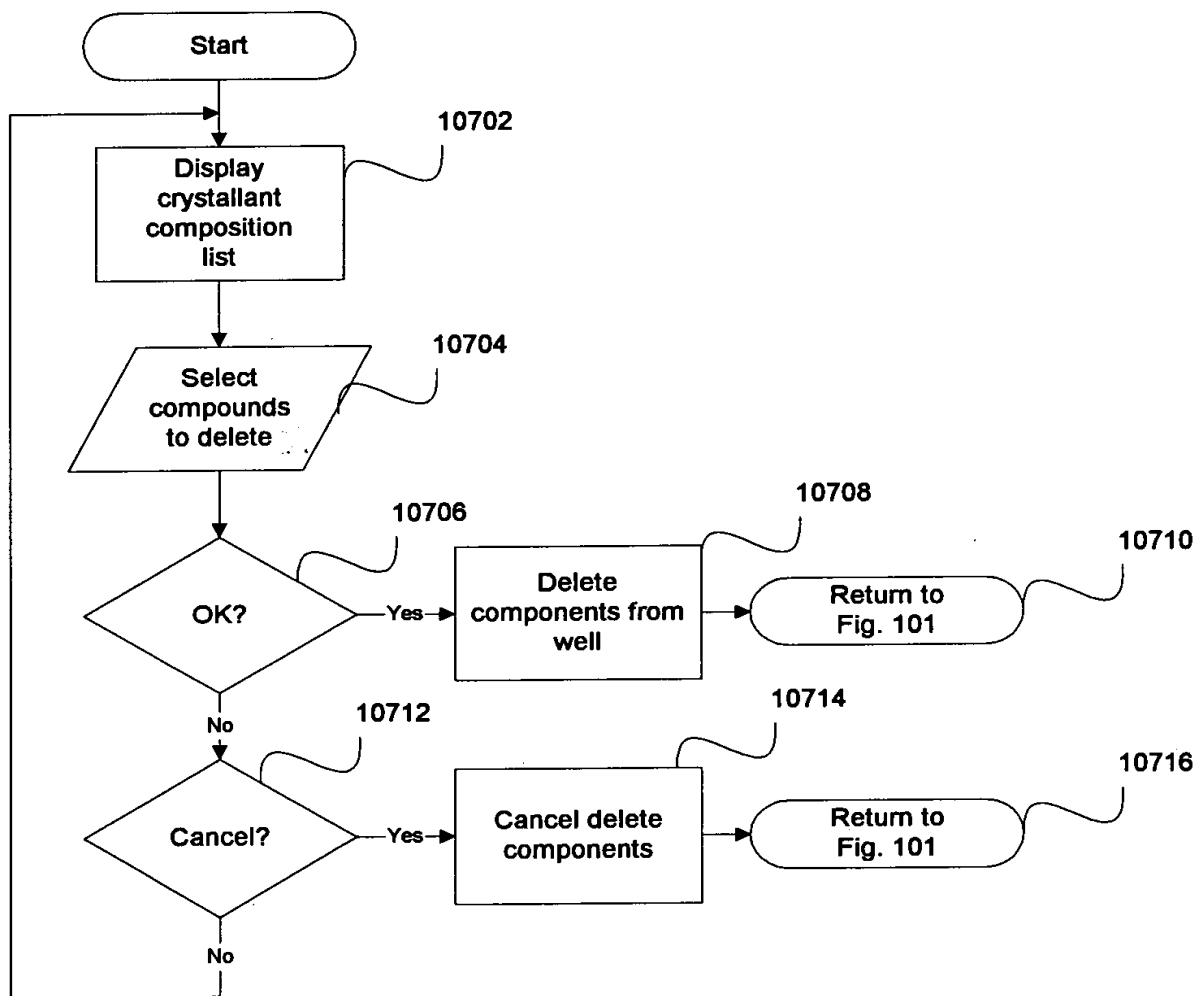


FIGURE 107



002080" 58T E 960

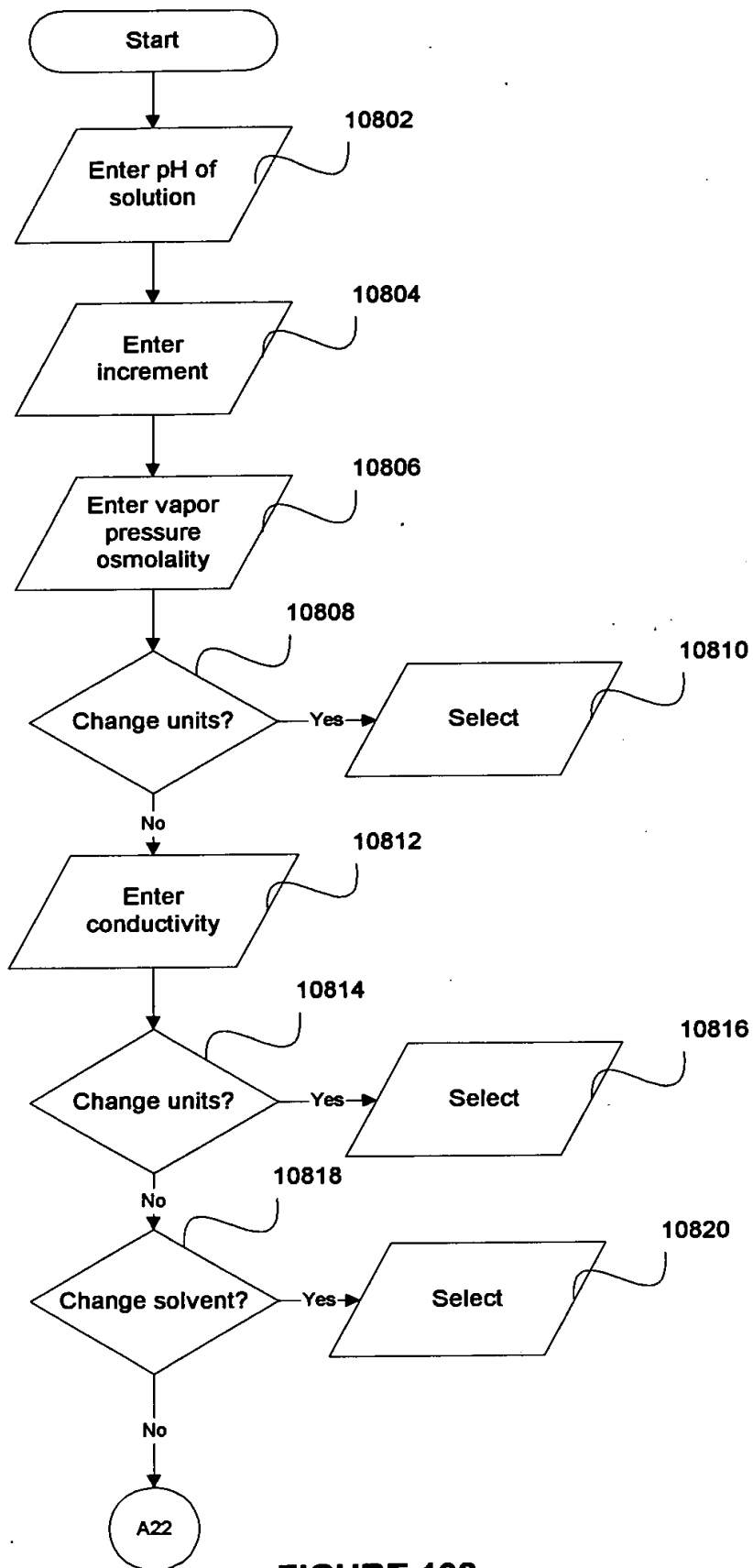


FIGURE 108

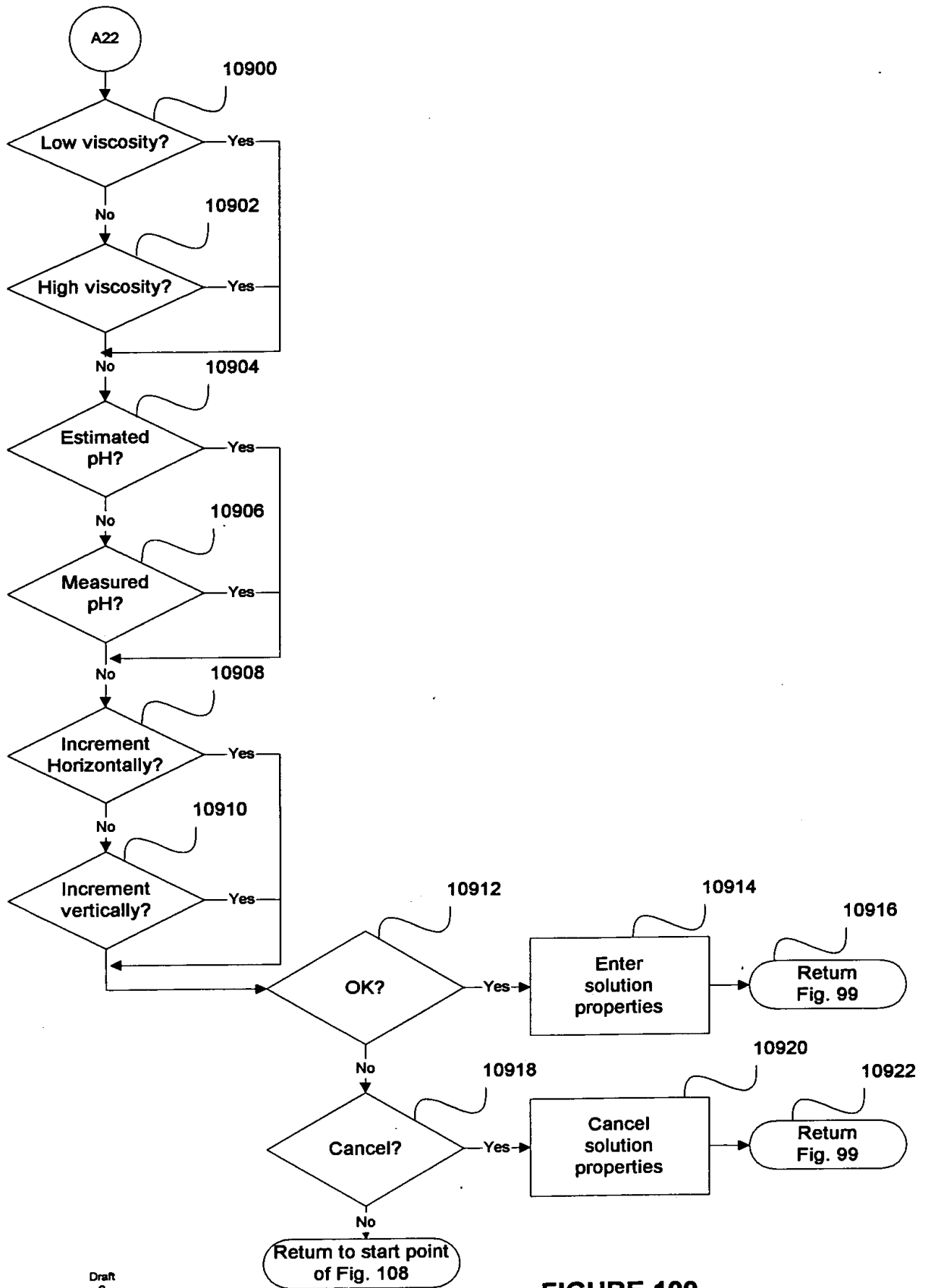


FIGURE 109

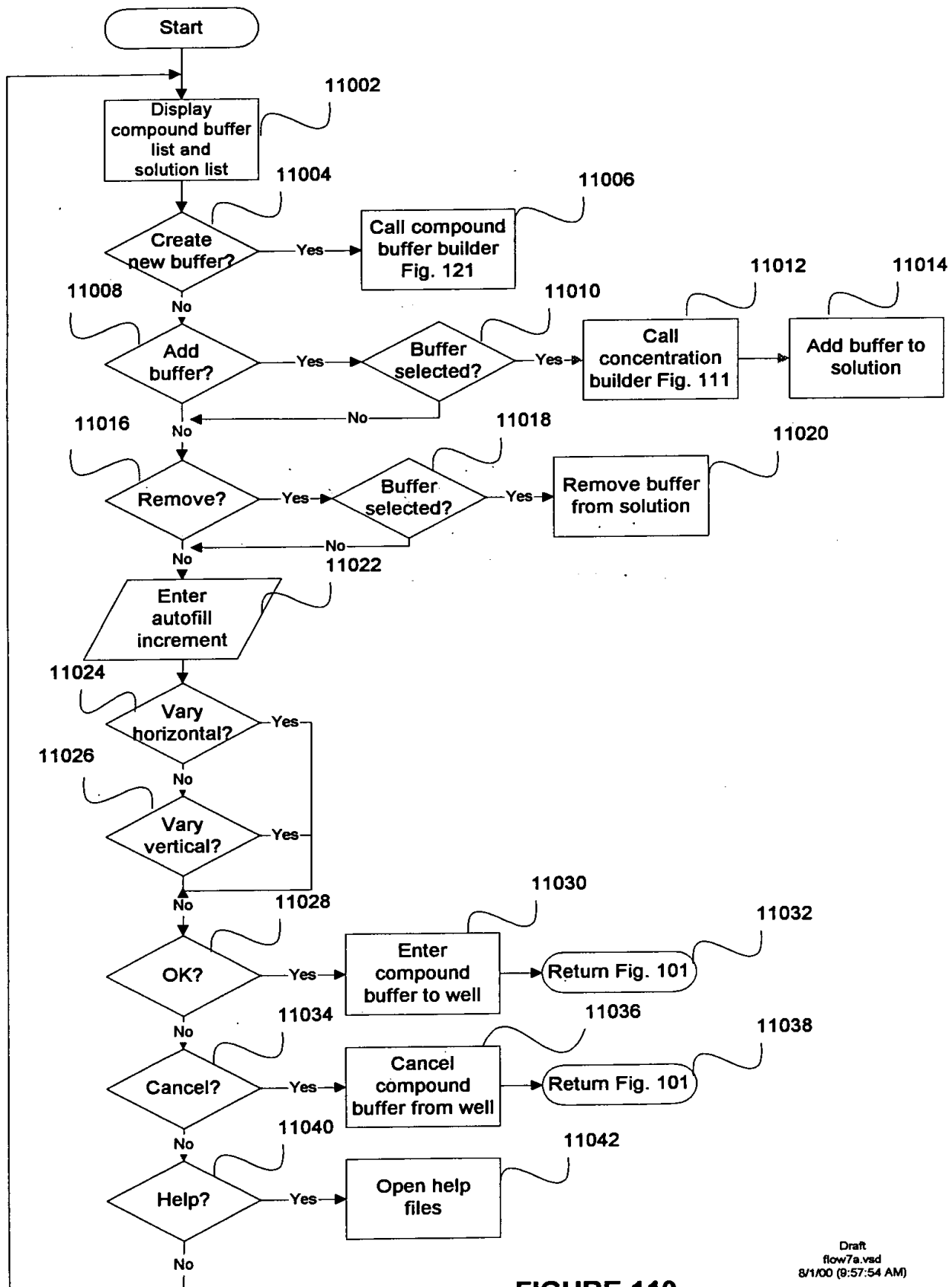


FIGURE 110

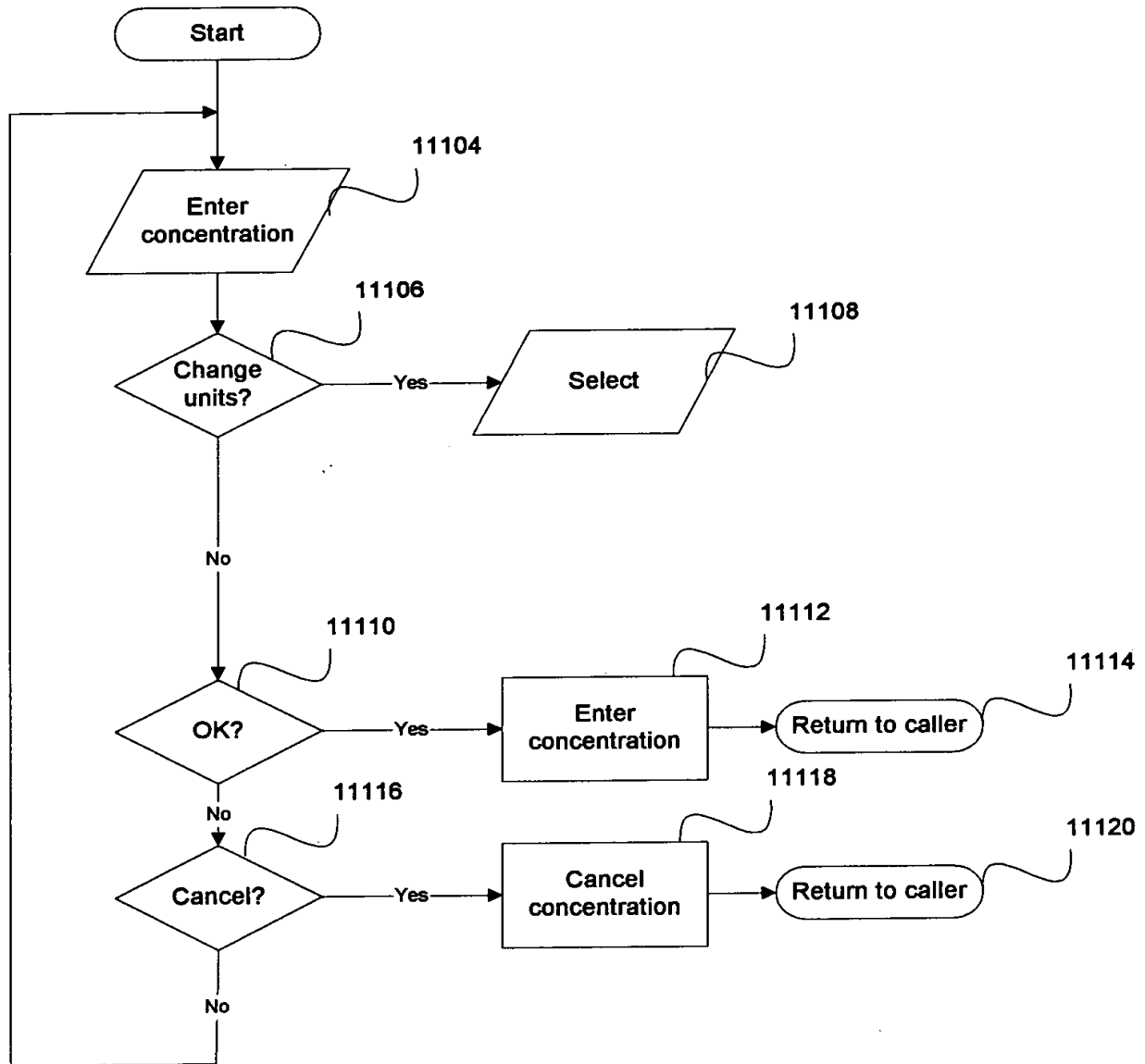
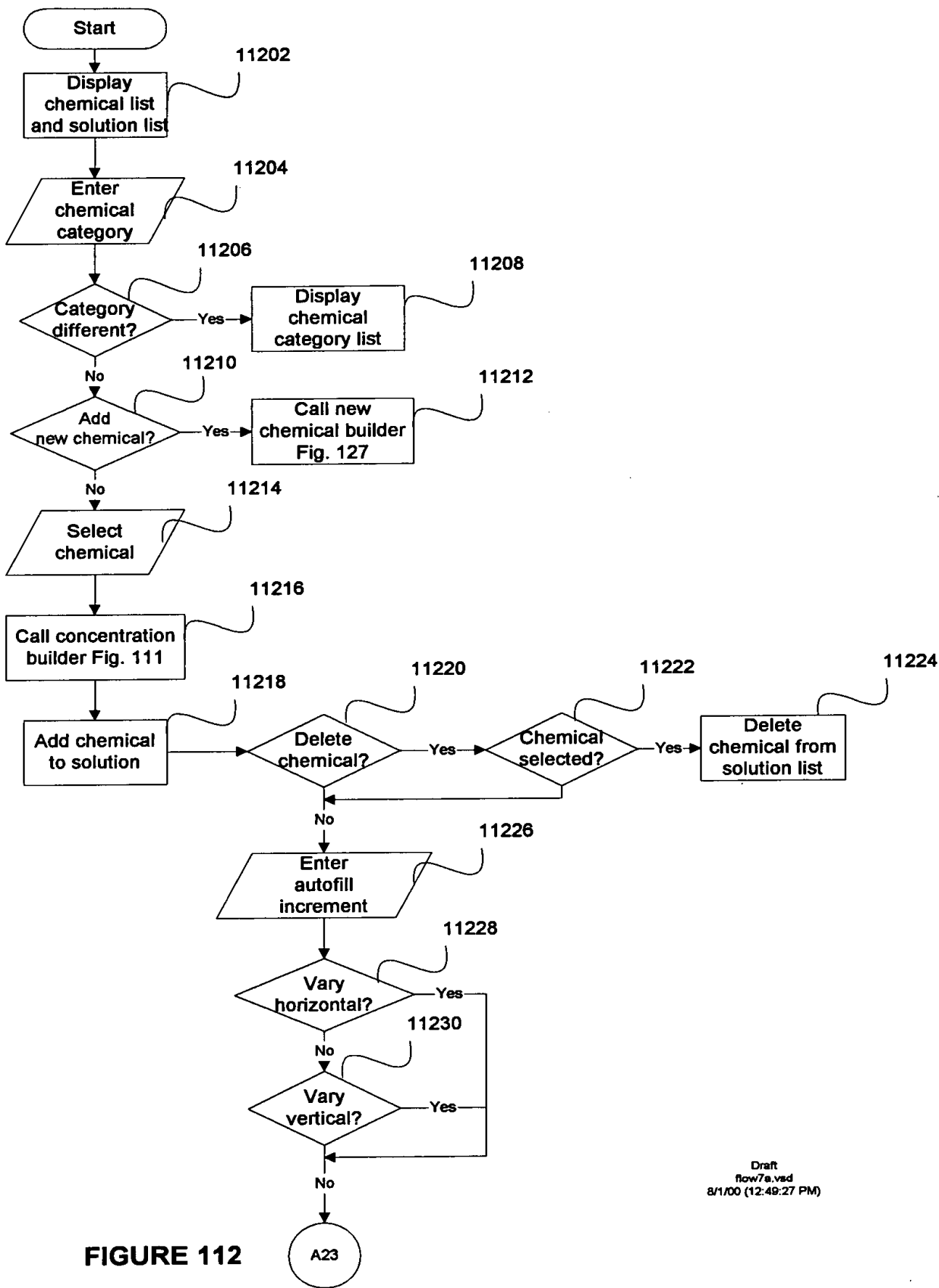


FIGURE 111

002080" 53T.E960



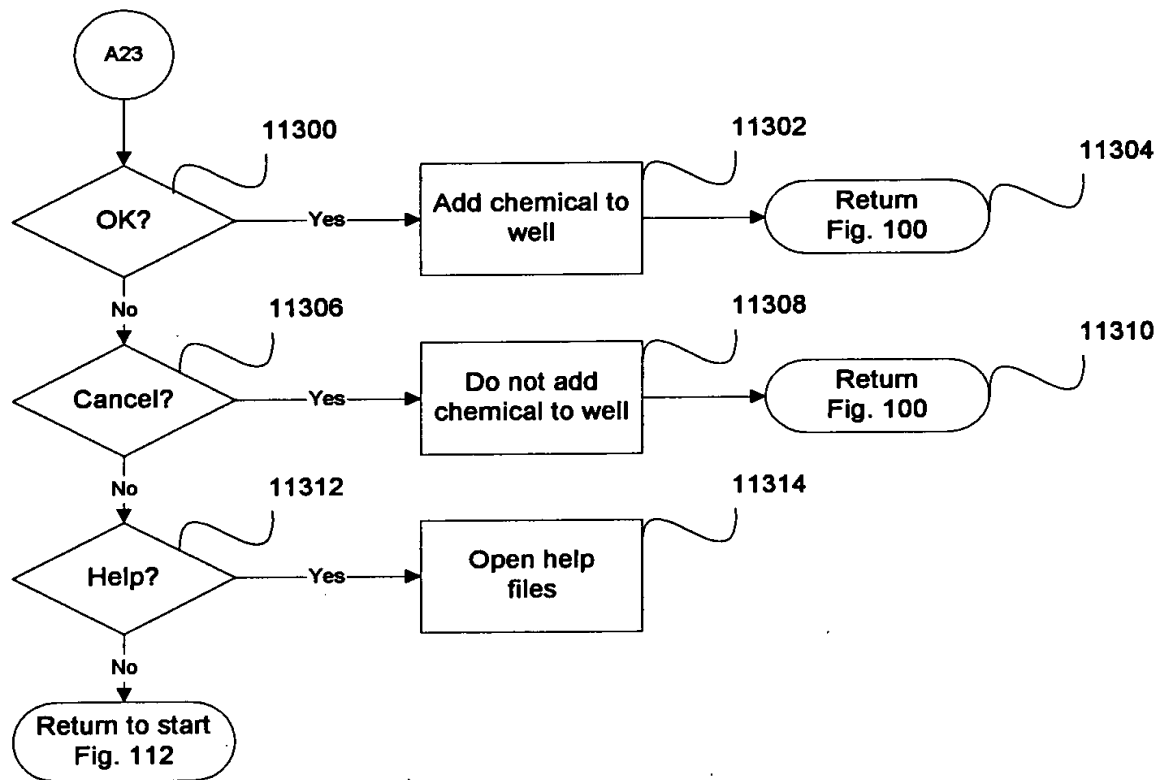


FIGURE 113

0961185.080200

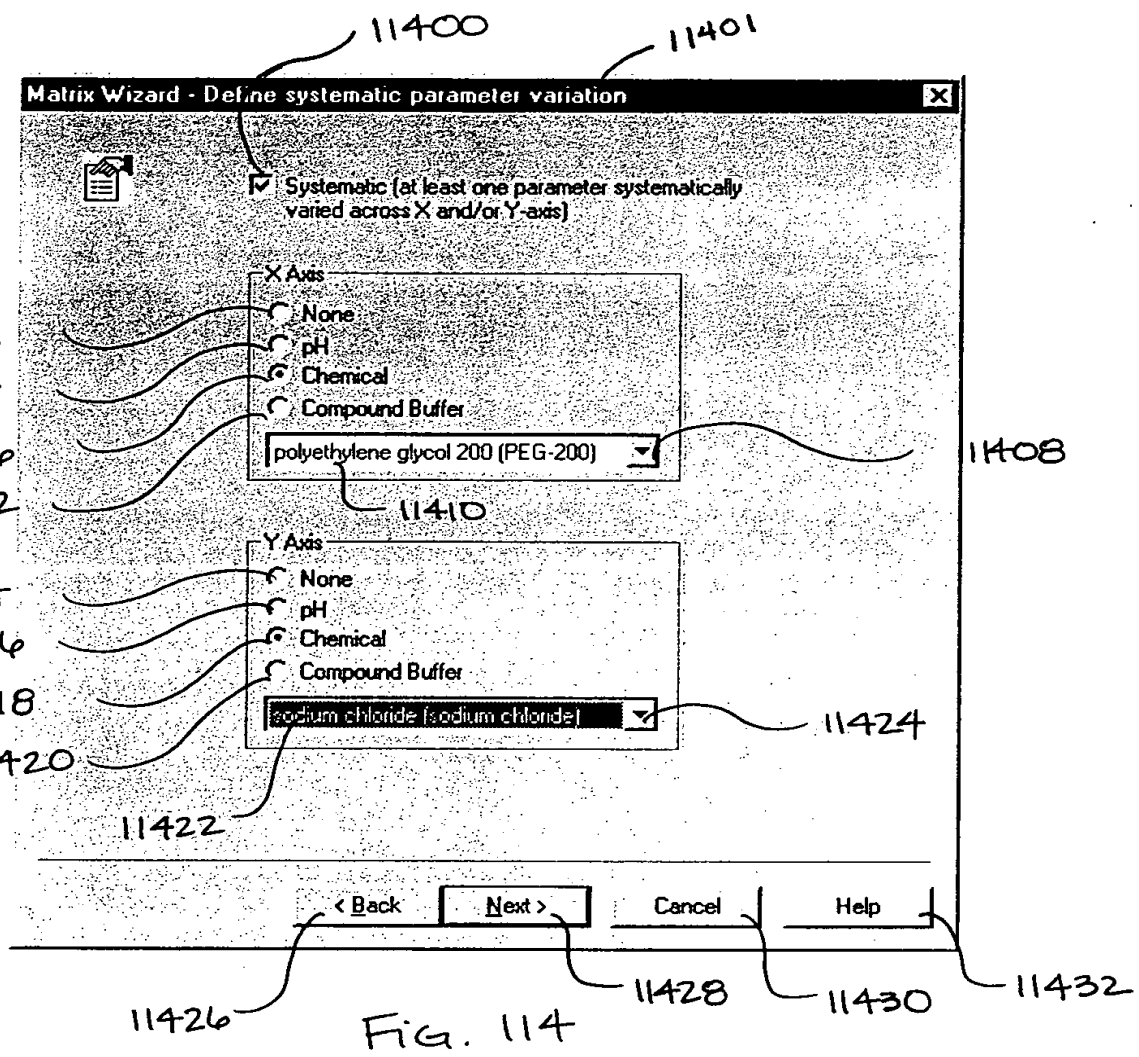
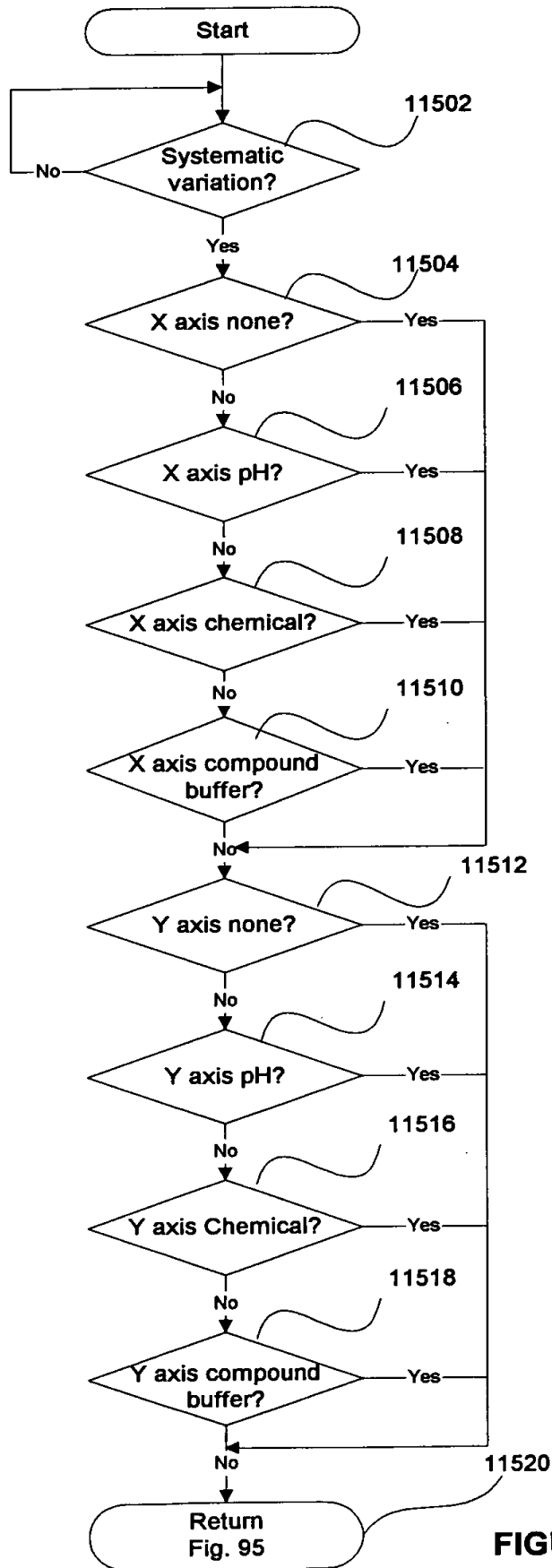


Fig. 114



**FIGURE 115**



002080" 58T'E'960

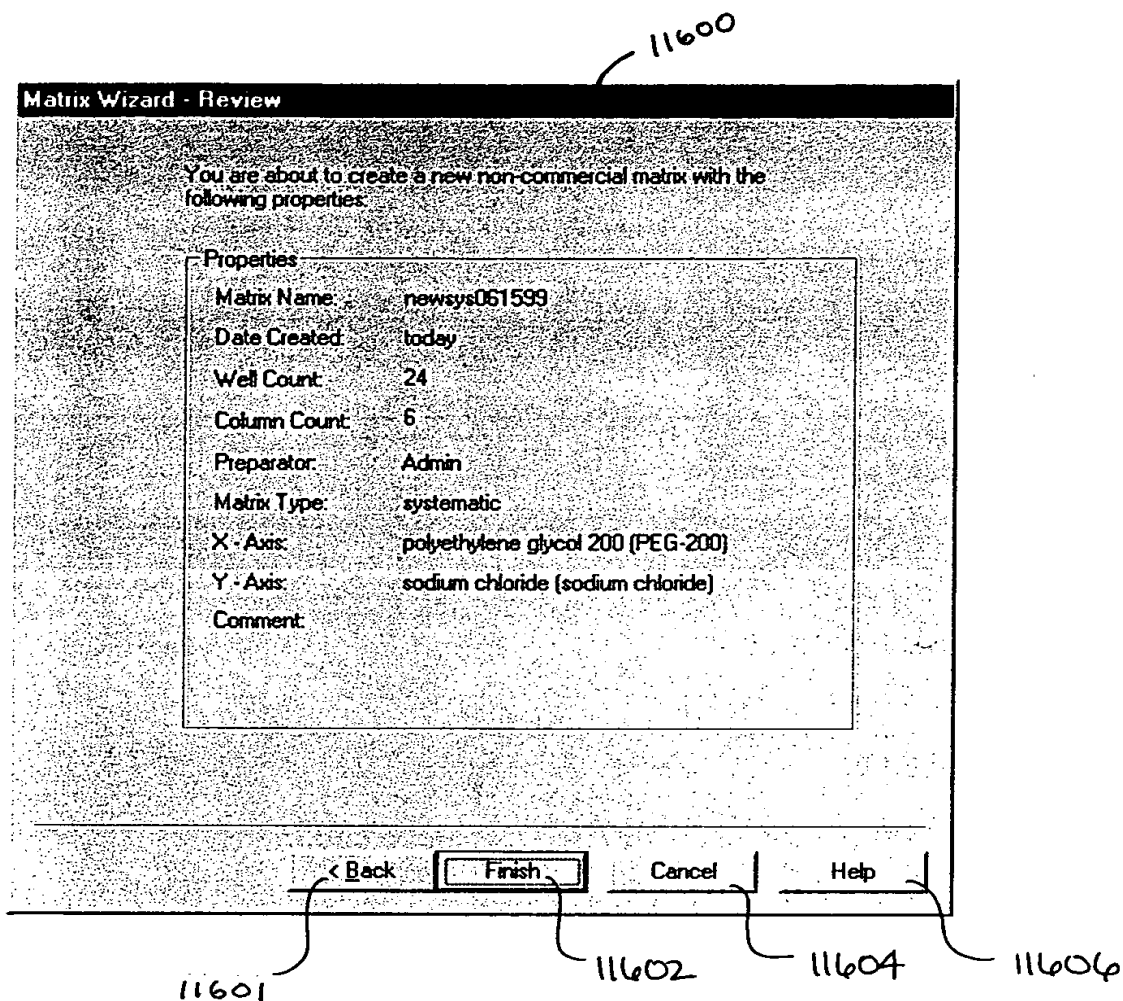
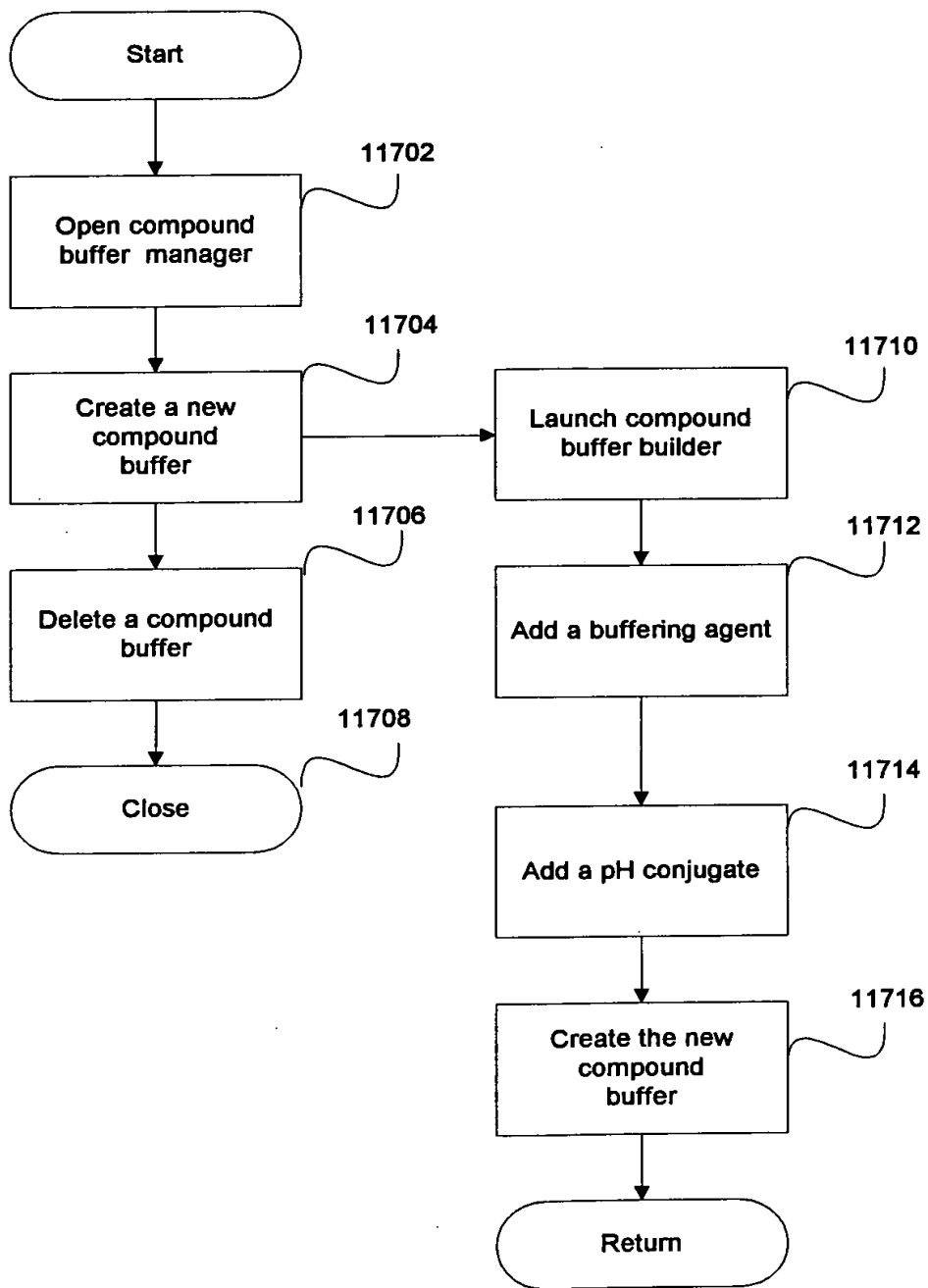


Fig. 116



**FIGURE 117**

H<sup>+</sup>

11800

002080-5512960

11801

### H<sup>+</sup> Compound Buffer Manager

Buffer PH	Buffering Agent (Full name)	Buf Agent (abbr)	Buf Agent (Mnft)
H <sup>+</sup> 4.20	sodium phosphate dibasic	Na2 H phosphate	Sigma Chemical
H <sup>+</sup> 4.50	acetic acid	acetic acid	Sigma Chemical
H <sup>+</sup> 4.60	sodium acetate trihydrate	NaAc	Hampton Research
H <sup>+</sup> 5.50	sodium cacodylic acid trihydrate	Na cacodylate	Hampton Research
H <sup>+</sup> 5.50	sodium citrate dihydrate	Na3 citrate	Sigma Chemical
H <sup>+</sup> 5.60	sodium citrate dihydrate	Na3 citrate	Hampton Research
H <sup>+</sup> 5.60	2-morpholinoethanesulfonic acid	MES	Hampton Research
H <sup>+</sup> 6.00	sodium cacodylic acid trihydrate	Na cacodylate	Hampton Research
H <sup>+</sup> 6.00	2-morpholinoethanesulfonic acid	MES	Hampton Research
H <sup>+</sup> 6.00	(2-N-morpholino)ethanesulfonic acid	MES	Sigma Chemical
H <sup>+</sup> 6.20	sodium phosphate dibasic	Na2 H phosphate	Sigma Chemical
H <sup>+</sup> 6.50	sodium dimethylarsinic acid	Na cacodylate	Sigma Chemical
H <sup>+</sup> 6.50	n-(2-acetamido)iminodiacetic acid	ADA	Hampton Research
H <sup>+</sup> 6.50	sodium citrate dihydrate	Na3 citrate	Hampton Research
H <sup>+</sup> 6.50	1,3-diaza-2,4-cyclopentadiene	imidazole	Hampton Research
H <sup>+</sup> 6.50	sodium cacodylic acid trihydrate	Na cacodylate	Hampton Research
H <sup>+</sup> 6.50	2-morpholinoethanesulfonic acid	MES	Hampton Research

New... 11808

Delete... 11802

Help... 11804

Close... 11806

Fig. 118

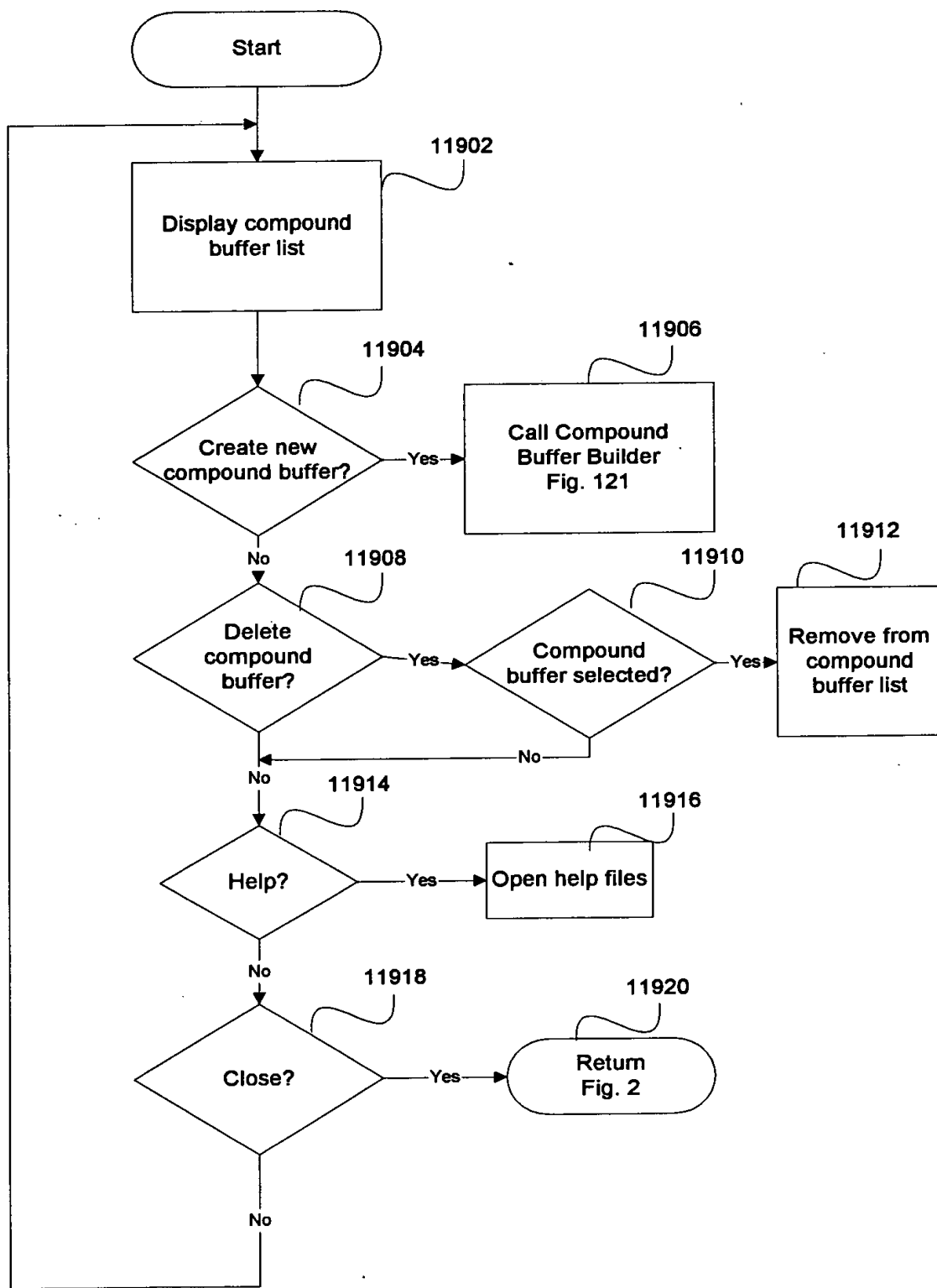


FIGURE 119

002080" 59T.E.960

12000

12006

12001

12002

12004

12008

12010

12012

12014

12016

12018

Compound Buffer Builder

Buffering Agent List

Chemical Name	Abbreviation
acetic acid	acetic acid
cetyl trimethylammonium bromide	CTAB
citric acid monohydrate	citric acid
di-sodium hydrogen phosphate, dibasic	Na2 H phosphate

pH Conjugate (Counter Ion) List

Chemical Name	Abbreviation
potassium dihydrogen phosphate, mon...	K H2 phosphate
sodium acetate	NaAc
sodium acetate trihydrate	NaAc
sodium cacodylic acid trihydrate	Na cacodylate

Compound Buffer

Buffering Agent:

Name: acetic acid  
Abbr: acetic acid (C2H4O2)  
Mass: 60.05 Da  
Mfctr: Sigma Chemical Co.

Counter Ion:

Name: sodium acetate  
Abbr: NaAc (NaC2H3O2)  
Mass: 82.03 Da  
Mfctr: Sigma Chemical Co.

Buffer pH [1..14]: 4.9

Comment: acetate buffer pH 4.9

Help

A Buffer is composed of exactly one Buffering Agent and exactly one pH Conjugate (Counter Ion). Double click on a Buffering Agent or pH Conjugate to copy the chemical to the right pane.

Commit

Cancel

Help...

FIG. 120

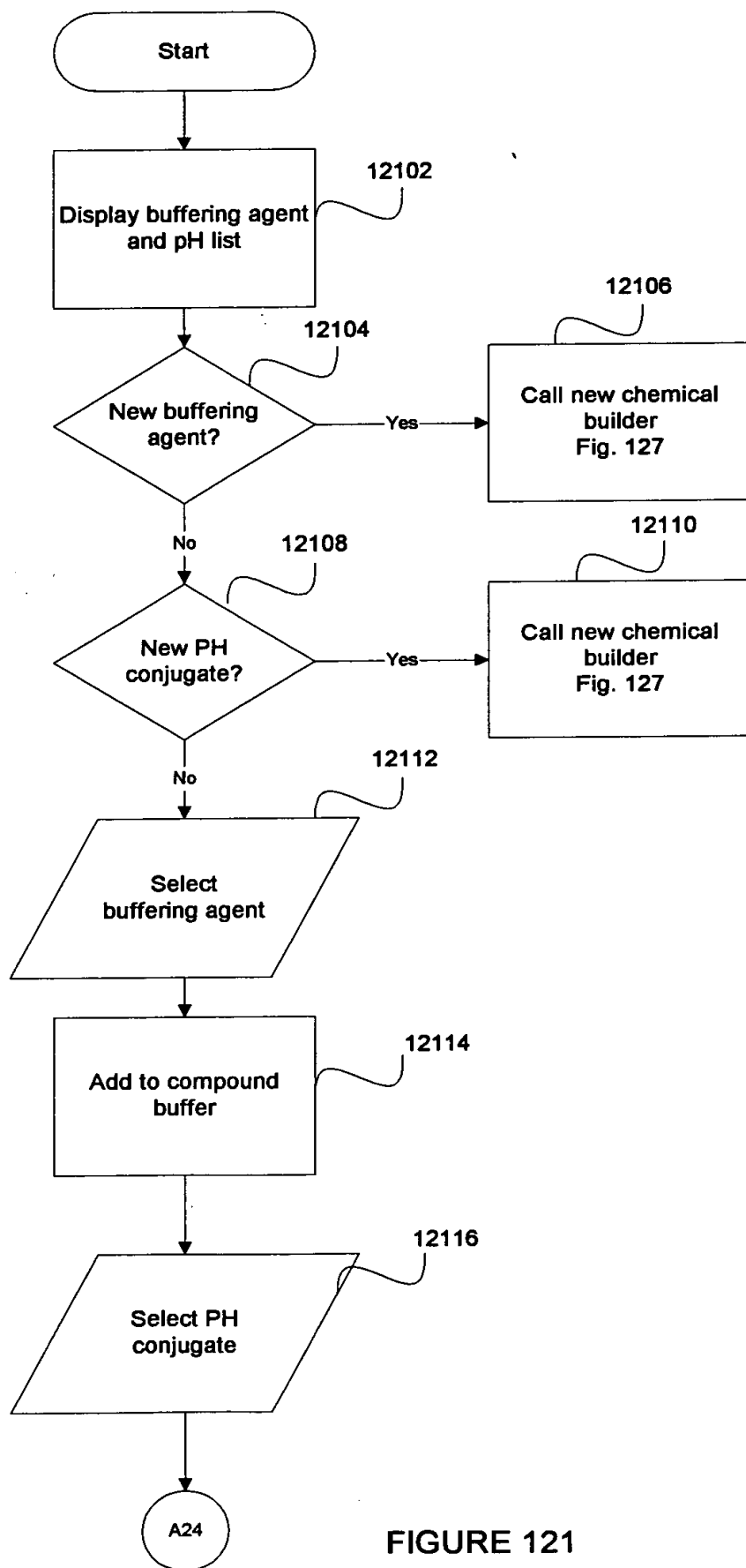


FIGURE 121

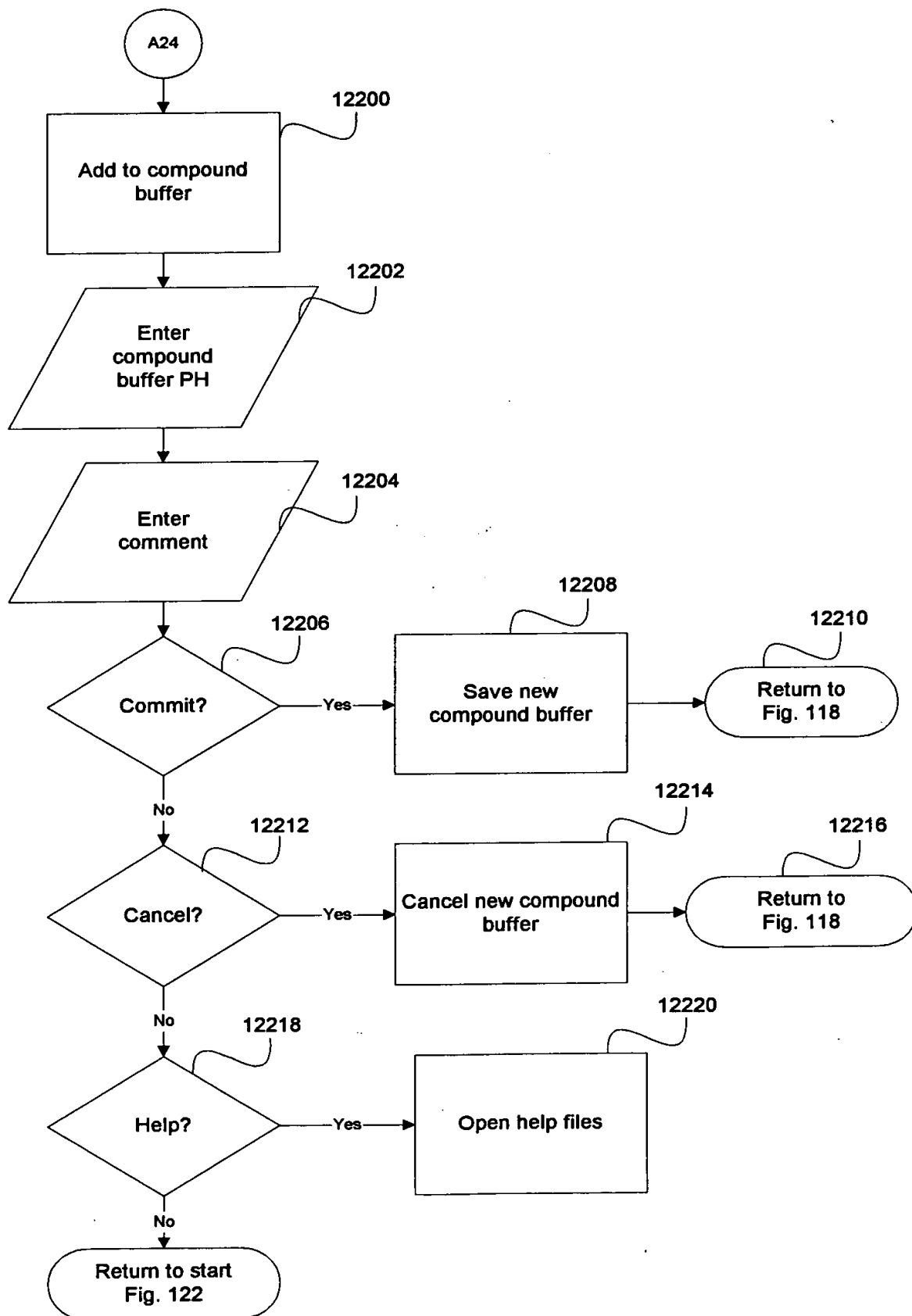
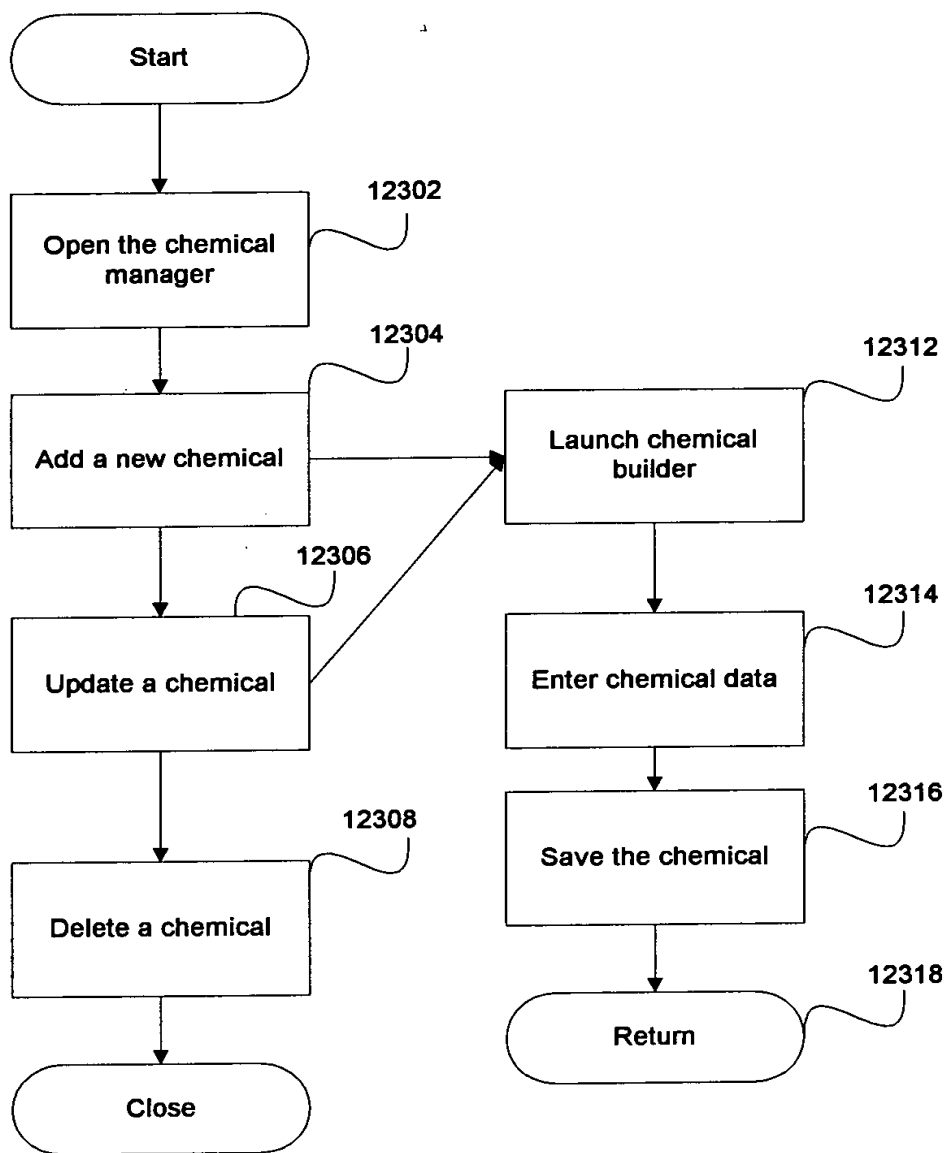


FIGURE 122



**FIGURE 123**





002080" 58TTE960

12400 12404 12406 12408

12401

## Chemical Manager

Category:

- Buffering Agent
- Chelator
- CryoCoolant
- CSI
- Detergent
- Gas
- HeavyAtomCompound
- Metal
- NucleationSuppressant
- Organic
- Other
- pHConjugate
- Precipitant**
- ReducingAgent
- Salt
- Solvent

New... Update... Delete Help...

Chemical Name	Abbr	Formula	Molecular Mass
1,2,3-heptanetriol	heptanetriol	C7H16O3	148.200 Da
1,2-propanediol	1,2-propanediol	C3H8O2	76.100 Da
1,2-propanediol	1,2-propanediol	C3H8O2	76.100 Da
1,4-butanediol	1,4-butanediol	C4H10O2	90.120 Da
1,4-dioxane	dioxane	C4H8O2	88.110 Da
1,6-hexanediol	hexanediol	C6H14O2	118.180 Da
2,5 hexanediol	hexanediol	CH3CH(OH)CH2...	118.180 Da
2,5-hexylene glycol	2,5-hexanediol	C6H14O2	118.180 Da
2-ethoxyethanol	2-ethoxyethanol	C4H10O2	90.120 Da
2-methyl-2,4-pentaned...	MPD	C6H14O2	118.180 Da
2-methyl-2,4-pentaned...	MPD	C6H14O2	118.180 Da
2-propanol	isopropanol	C3H8O	60.100 Da
2-propanol	isopropanol	C3H8O	60.100 Da
2-propanol	isopropanol	C3H8O	60.100 Da
2-propanol	isopropanol	C3H8O	60.100 Da

12410 12402

Select a chemical and click one of the top buttons or double click on a chemical to update.

Close 12412

Fig. 124

12501 12510

12501 12502 12504 12506 12514 12516 12522 12524

**New Chemical**

Name: ammonium sulfate

Abbr: (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>

Formula: (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>

Mass: 132.1 Da

Chemical Type: Precipitant

Density [g/ml]:

Manufacturer: Sigma Chemical Co.

Catalog: A4915

CAS: 7783-20-2

State

☐ Gas

☐ Liquid

☒ Solid

12524p

12512 12508 12520 12518

STOP

Warning

Catalog and CAS cannot be updated, once they have been entered, since they are the primary key for the chemical entity.

OK

Cancel

12528 12530

FIG. 125

002080-587E950

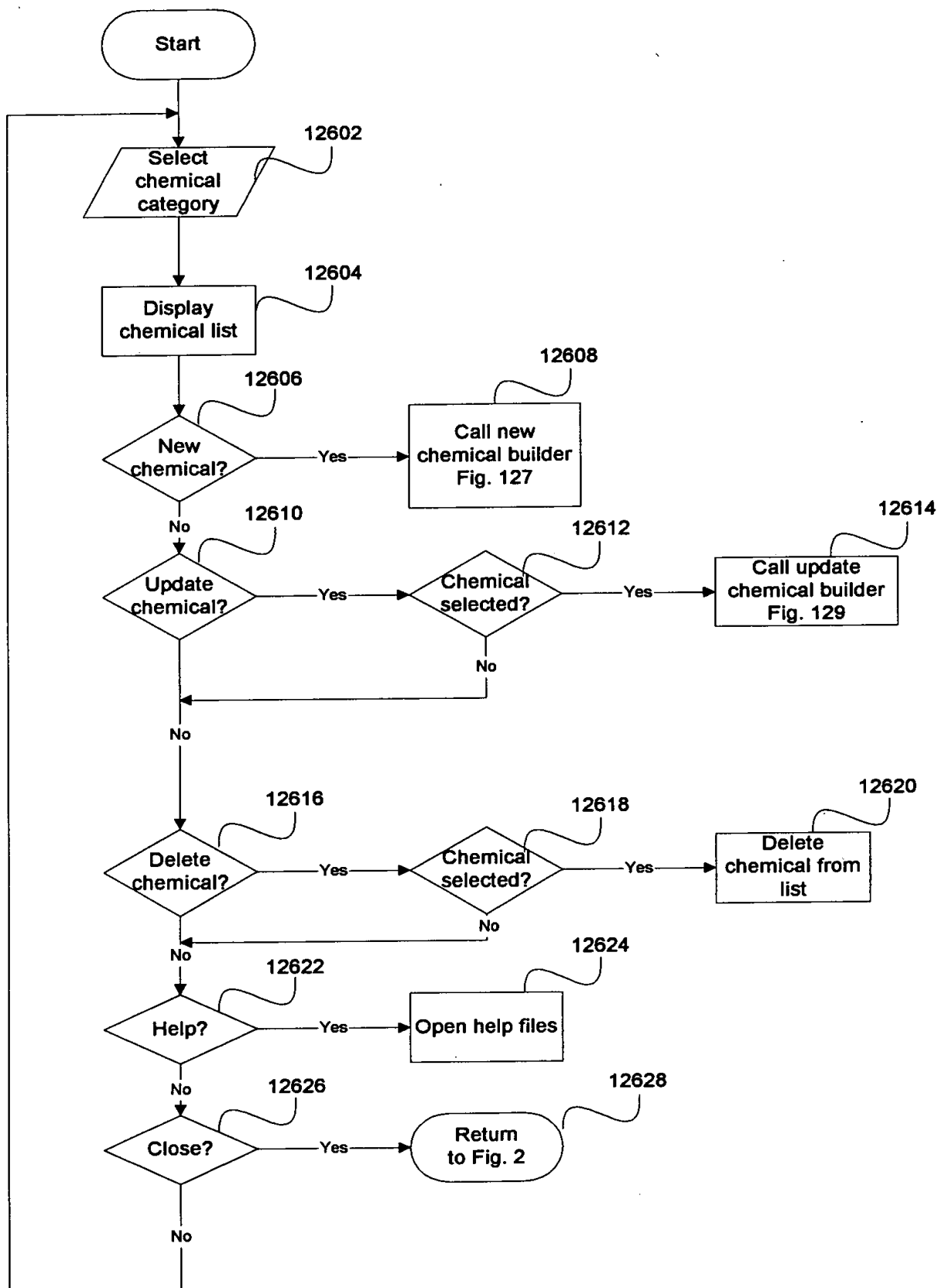


FIGURE 126

002080" 58TTC960

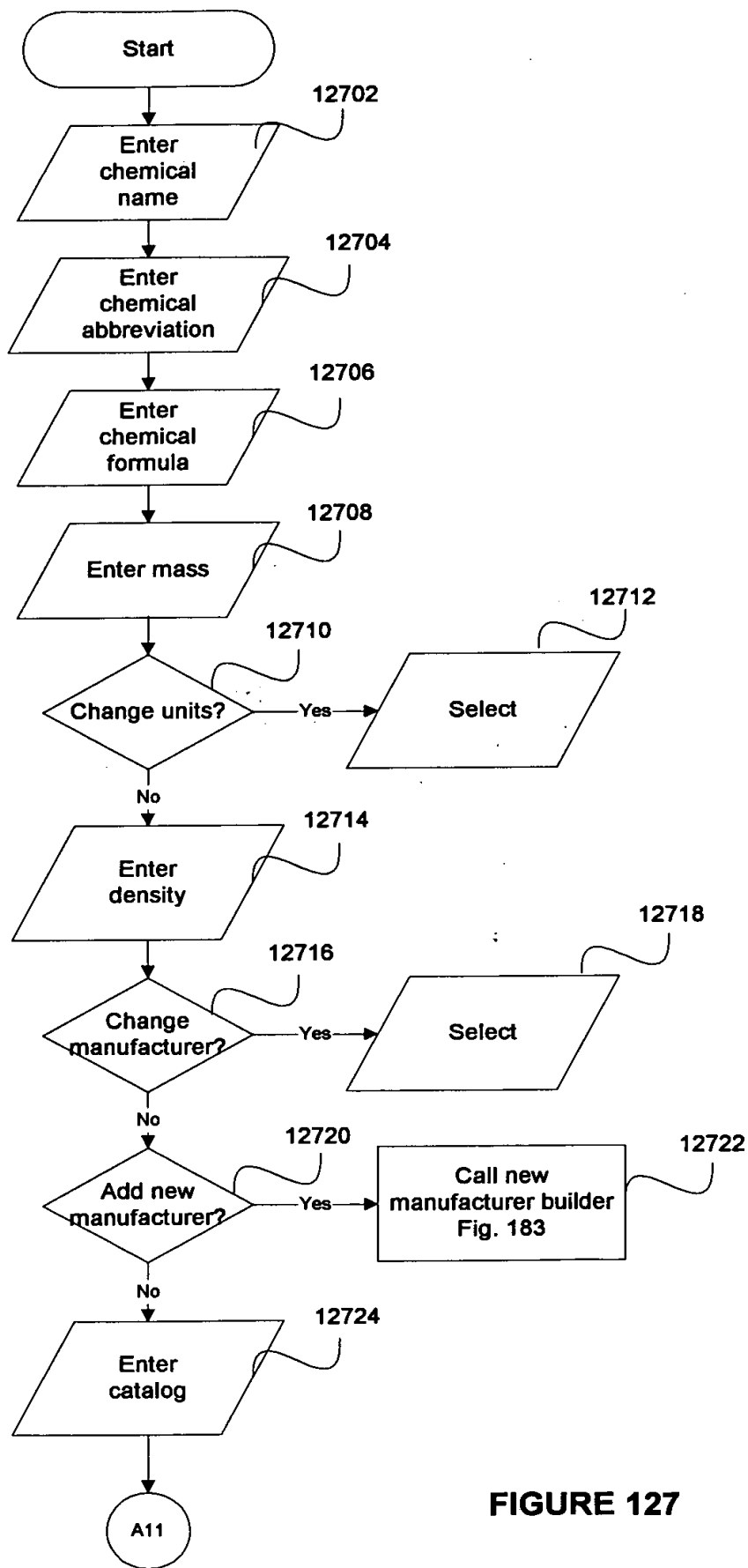


FIGURE 127

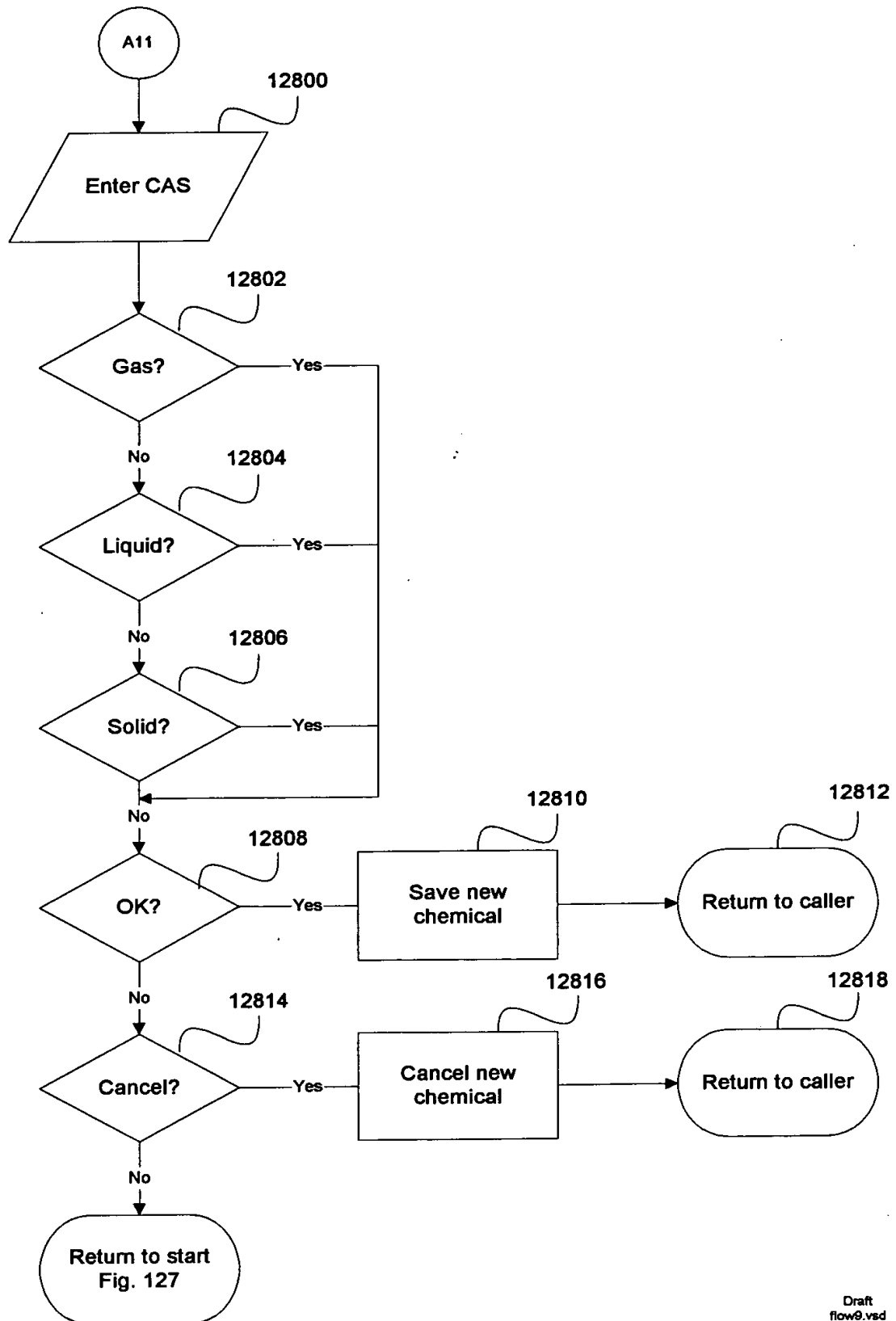


FIGURE 128

002030" 58TTC960

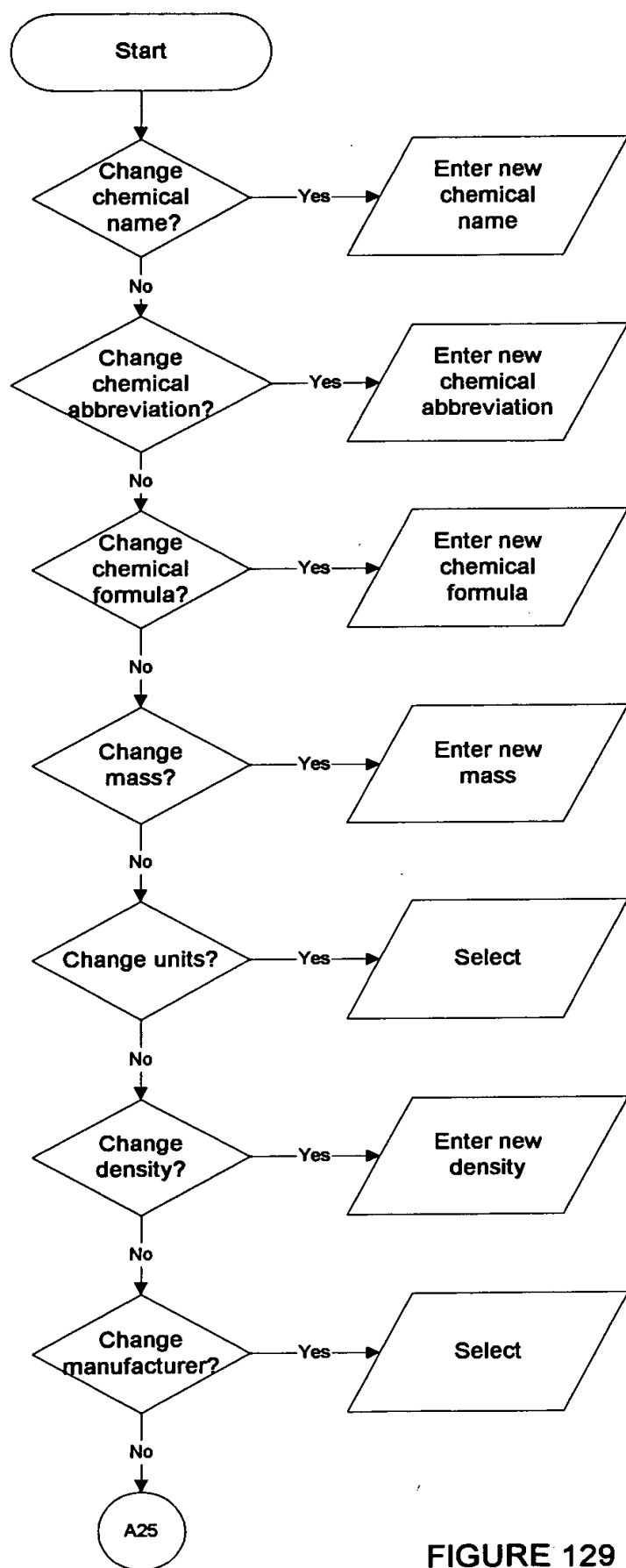


FIGURE 129

002080" 587E960

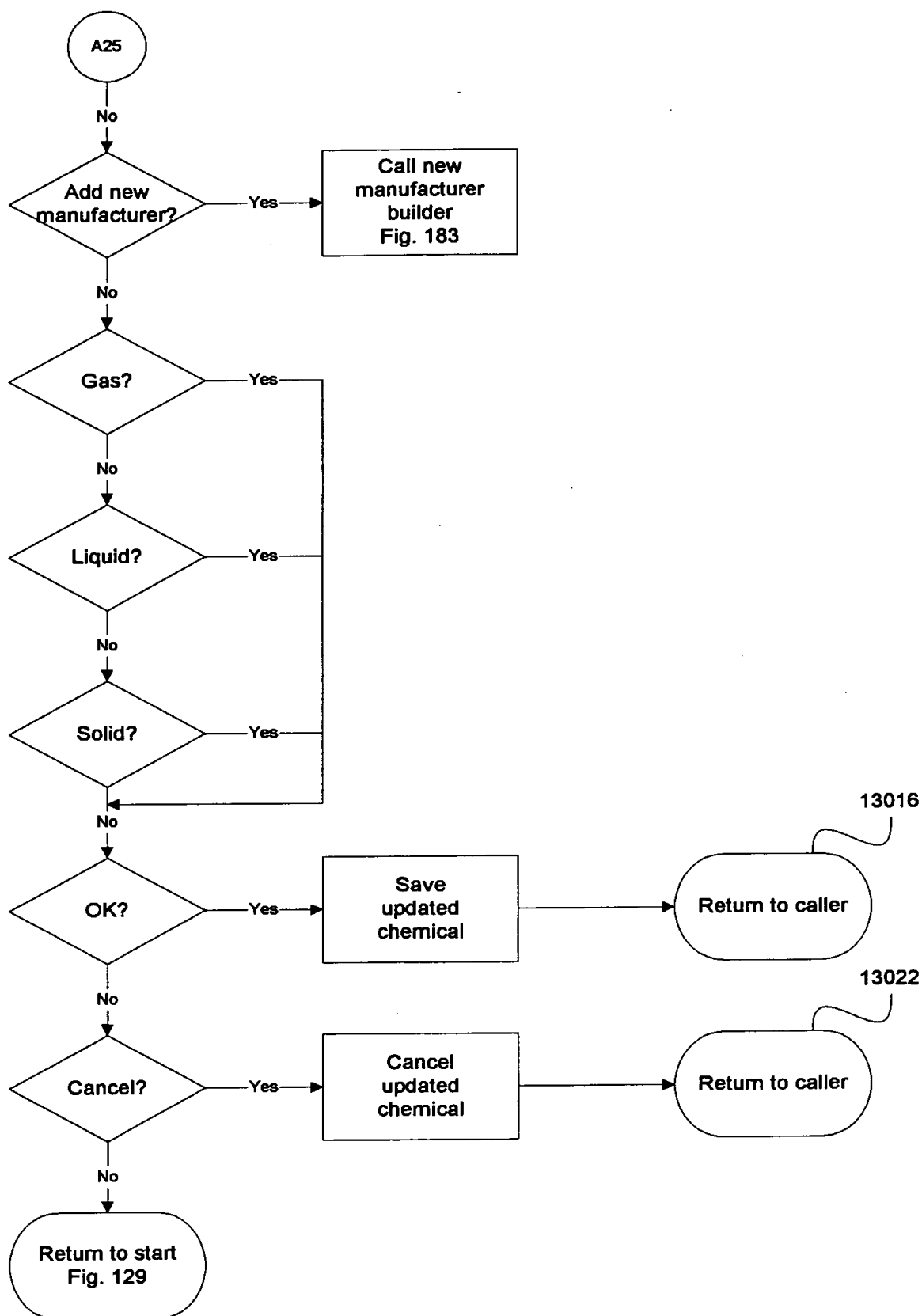


FIGURE 130

002090" 5371E350

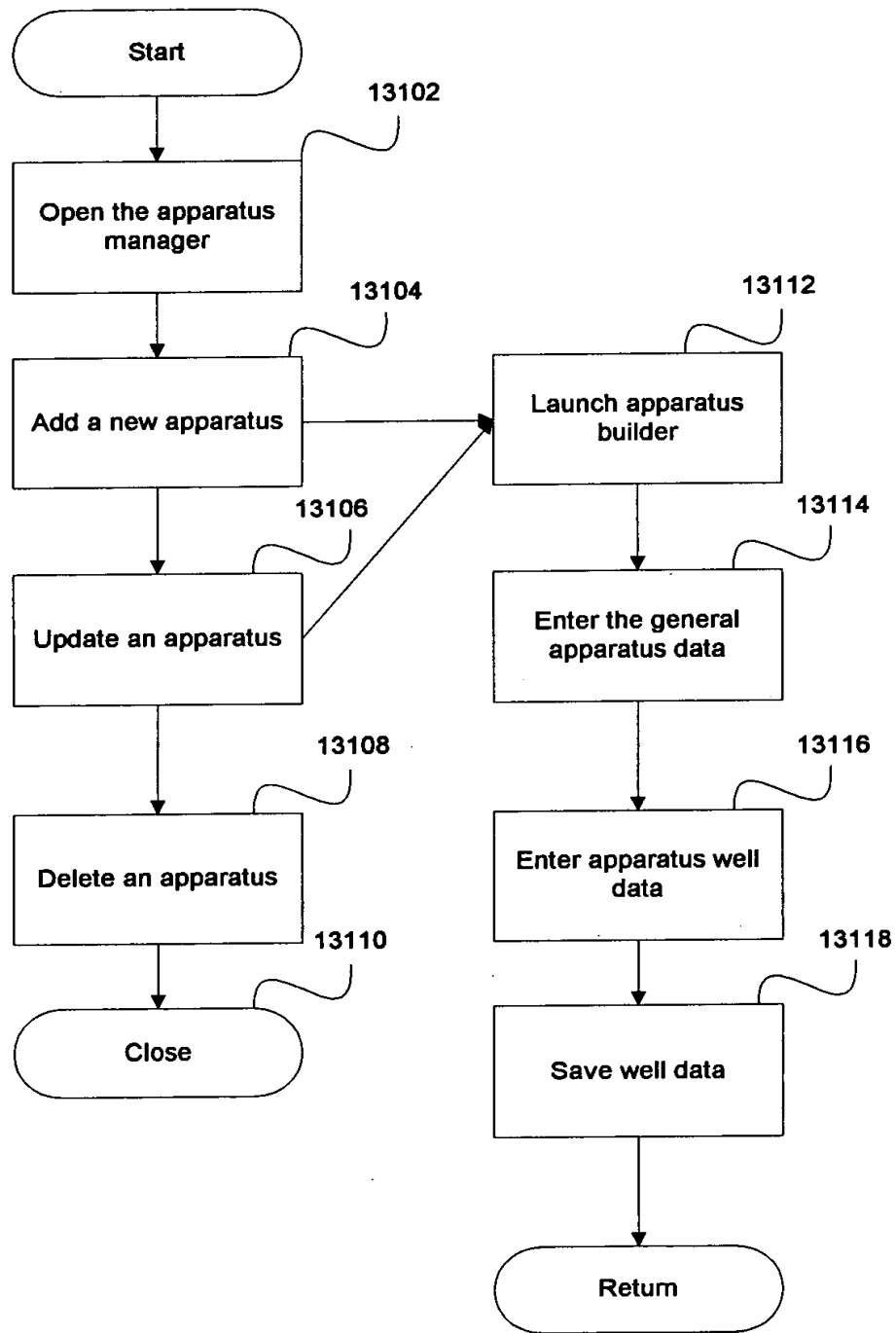


FIGURE 131



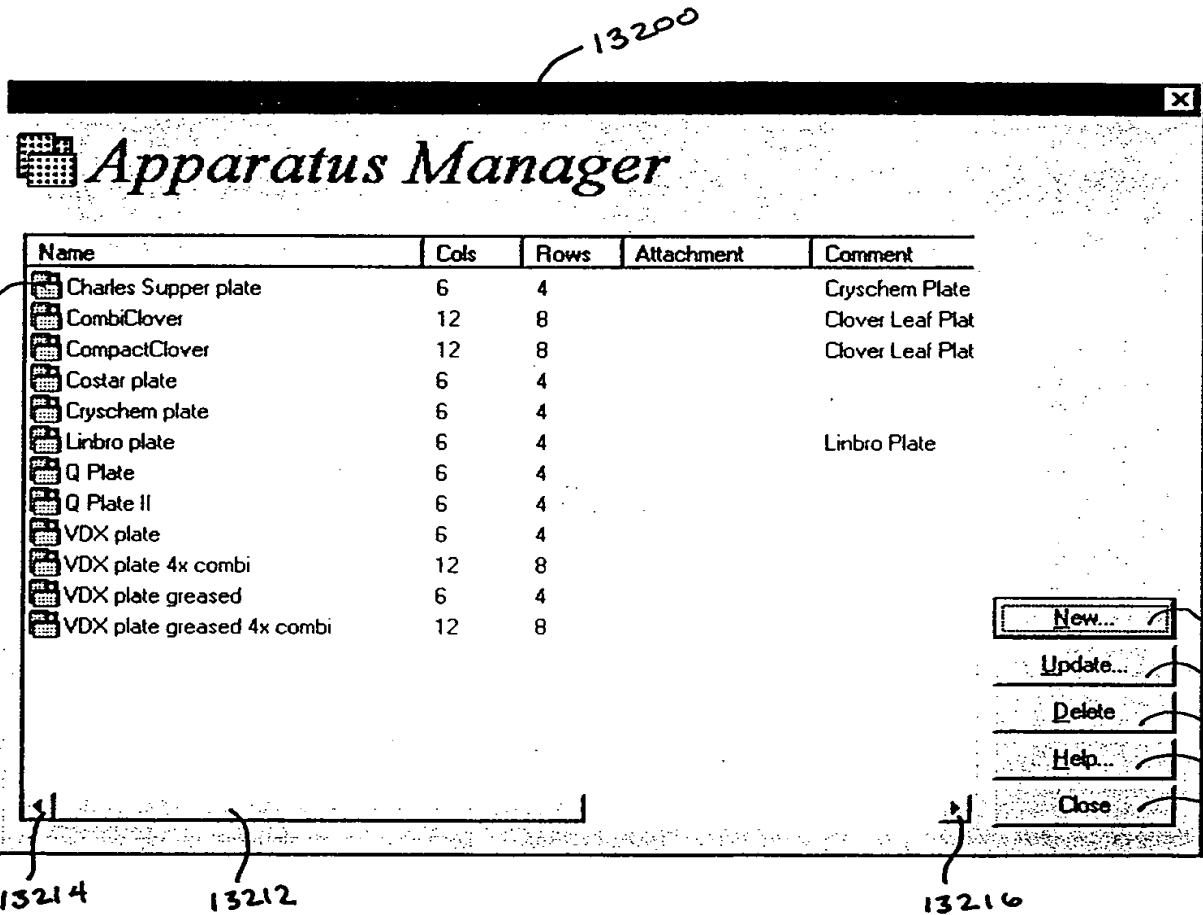


Fig. 132

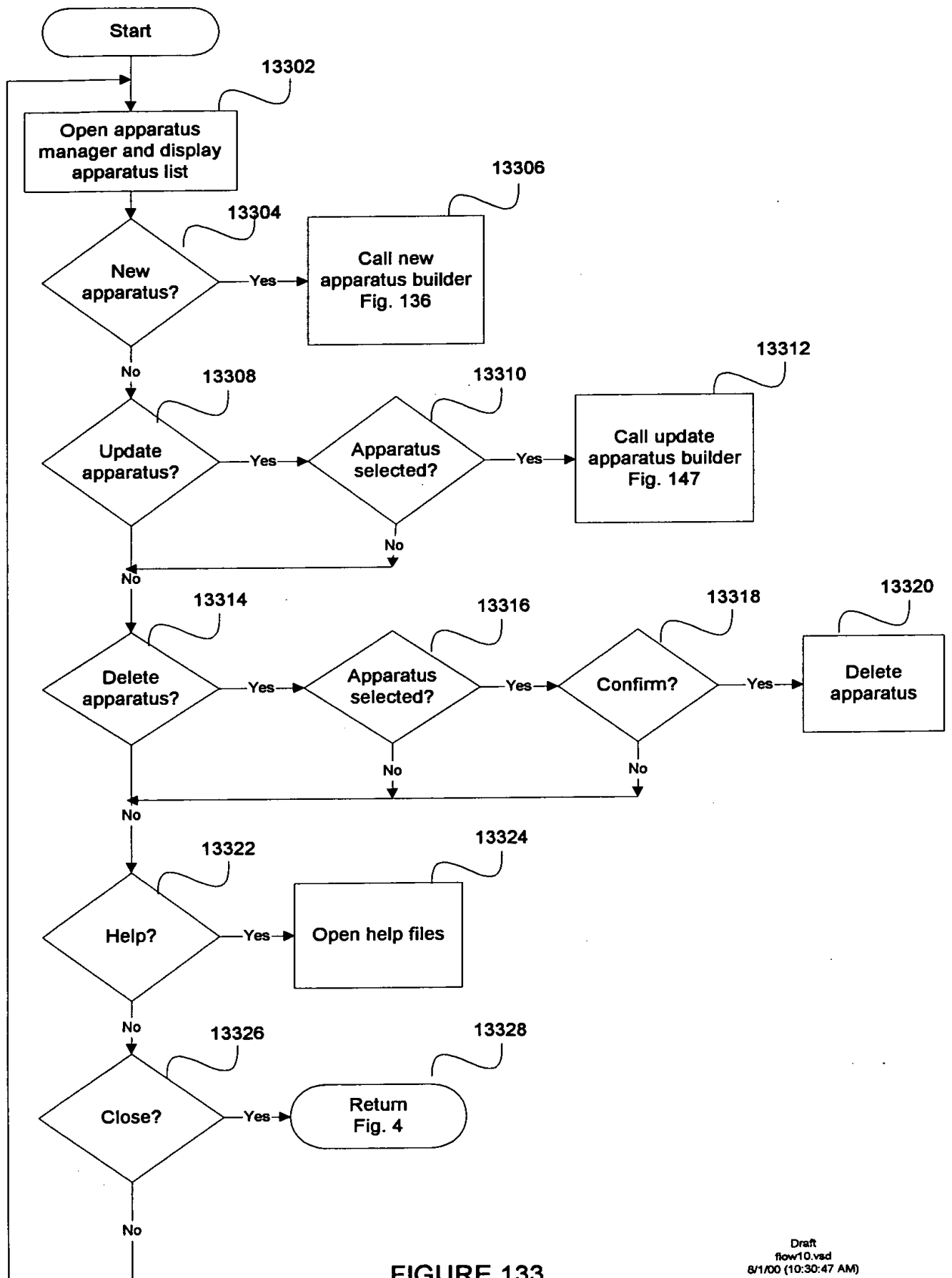


FIGURE 133

002080"58TTE960

13401 13402 13400

New Apparatus [X]

General apparatus data | Apparatus well data

13404 Name: CombiClover Jr.

13406 13410 Manufacturer: Emerald BioStructures, Inc. 13408

Columns: 8 Rows: 6 13419 E:\crymon\Help\crystalmonitor\images\coml

13414 Type: ☒ Crystallization 13412 ☐ Tube Rack

Base dim (x,y,z): 112 75 20

13418 Comment: 48-well CombiClover Jr. plate with standard microtiter plate footprint

Help  
For more detailed help, please click the help button.

OK Cancel Help... 13424

13420 13422

FIG. 134

002080" 5877E960

13500

**New Apparatus** [X]

General apparatus data | Apparatus well data

AutoFill... 13501

1 x y z Drop: Res: Drop Diameter: Res Diameter: Max Vol Drop: Max Vol Res:	2 x y z Drop: Res: Drop Diameter: Res Diameter: Max Vol Drop: Max Vol Res:	3 x y z Drop: Res: Drop Diameter: Res Diameter: Max Vol Drop: Max Vol Res:	4 x y Drop: Res: Drop Diameter: Res Diameter: Max Vol Drop: Max Vol Res:
9 x y z Drop: Res: Drop Diameter: Res Diameter: Max Vol Drop: Max Vol Res:	10 x y z Drop: Res: Drop Diameter: Res Diameter: Max Vol Drop: Max Vol Res:	11 x y z Drop: Res: Drop Diameter: Res Diameter: Max Vol Drop: Max Vol Res:	12 x y Drop: Res: Drop Diameter: Res Diameter: Max Vol Drop: Max Vol Res:
17 x y z Drop:	18 x y z Drop:	19 x y z Drop:	20 x y Drop:

13506

OK Cancel Help... 13502 13504

FIG. 135

09631185-080200

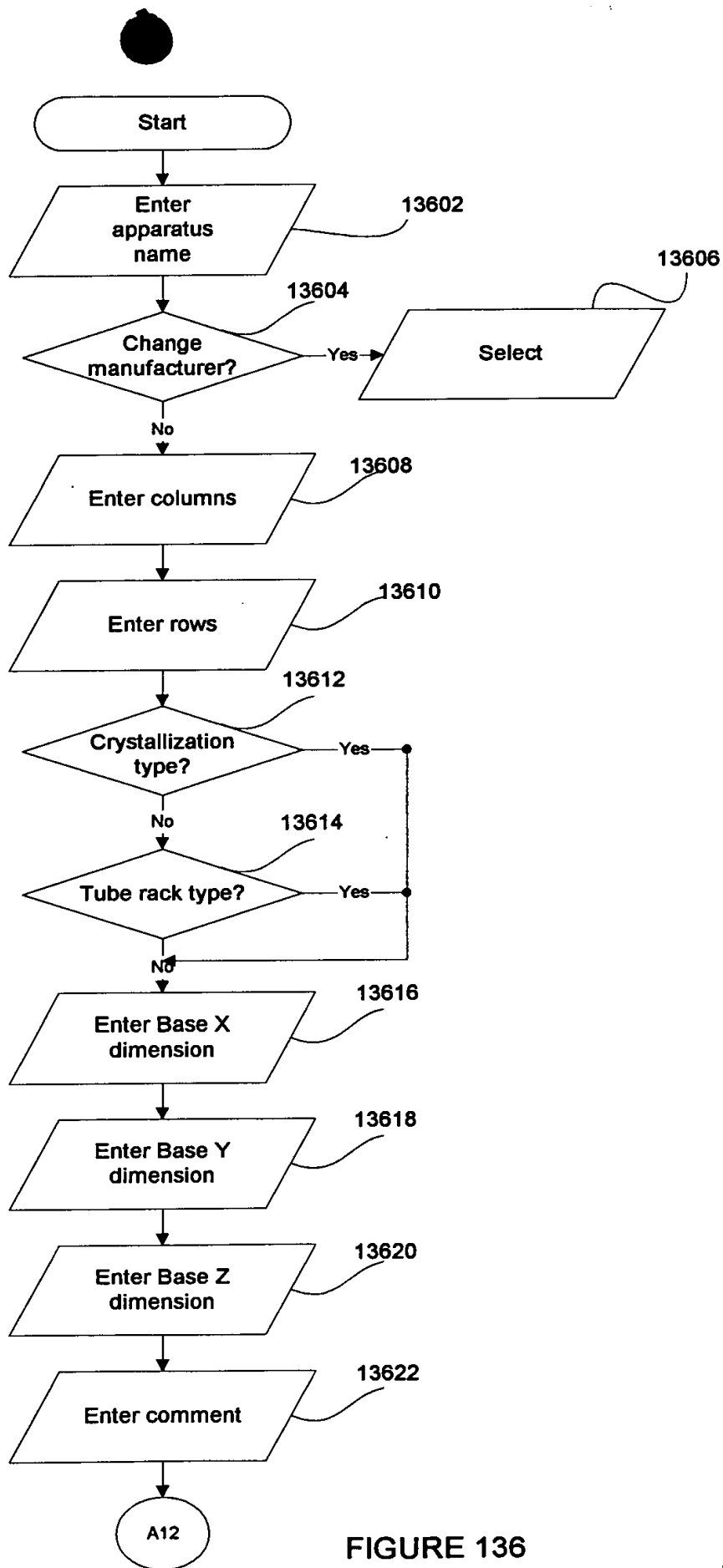


FIGURE 136

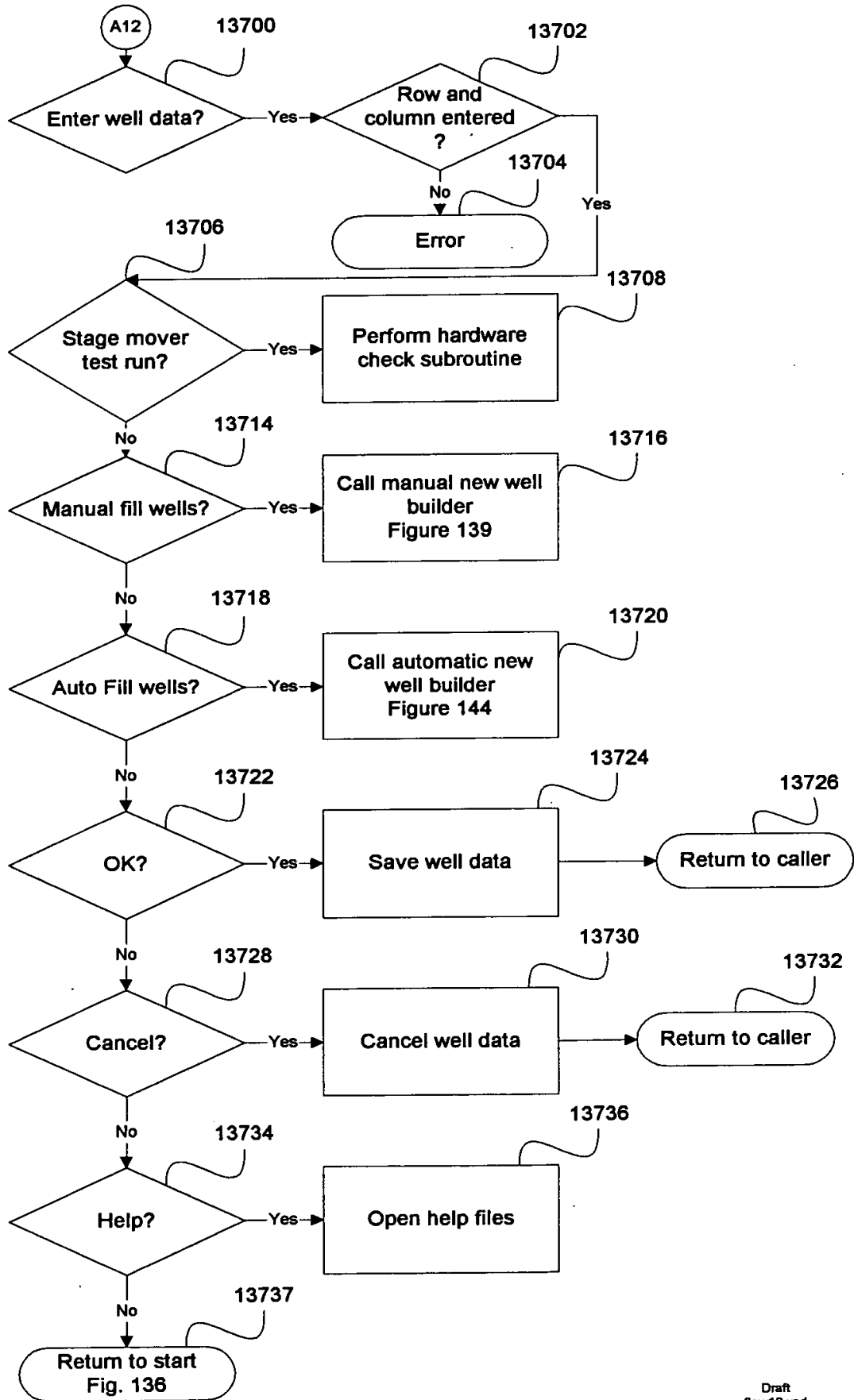


FIGURE 137

13800

Updating Well # 1
✕

Well coordinates in millimeter (mm)

	X	Y	Z	Diameter
Drop chamber:	10	5	5	5
Res. Chamber:	15	10	20	10

Volume

Max Vol Drop Chamber:	30	μl	<input checked="" type="checkbox"/>
Max Vol Res. Chamber:	1000	μl	<input checked="" type="checkbox"/>

Help...
OK
Cancel

FIG. 138

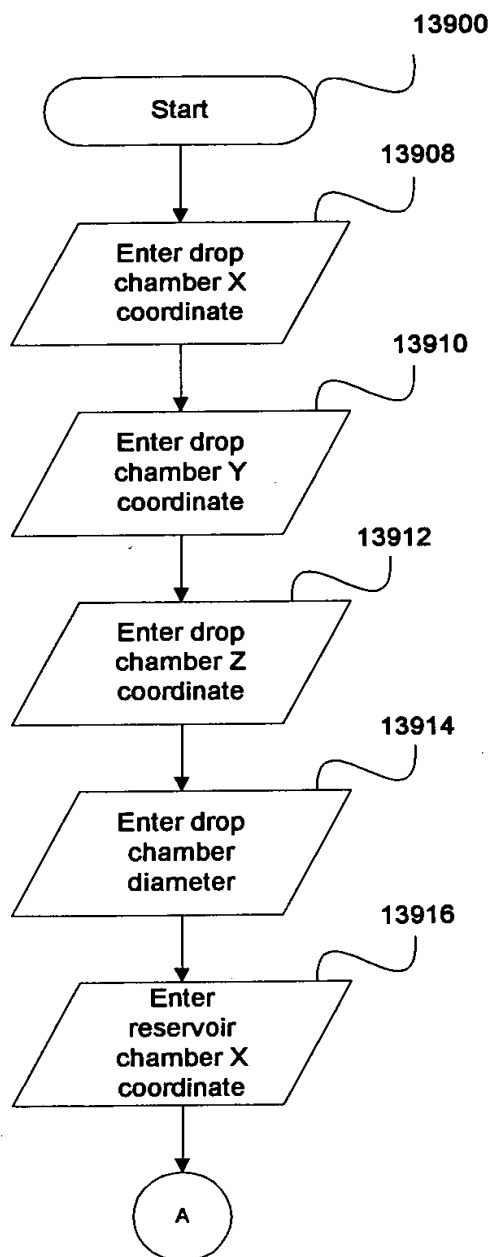


FIGURE 139



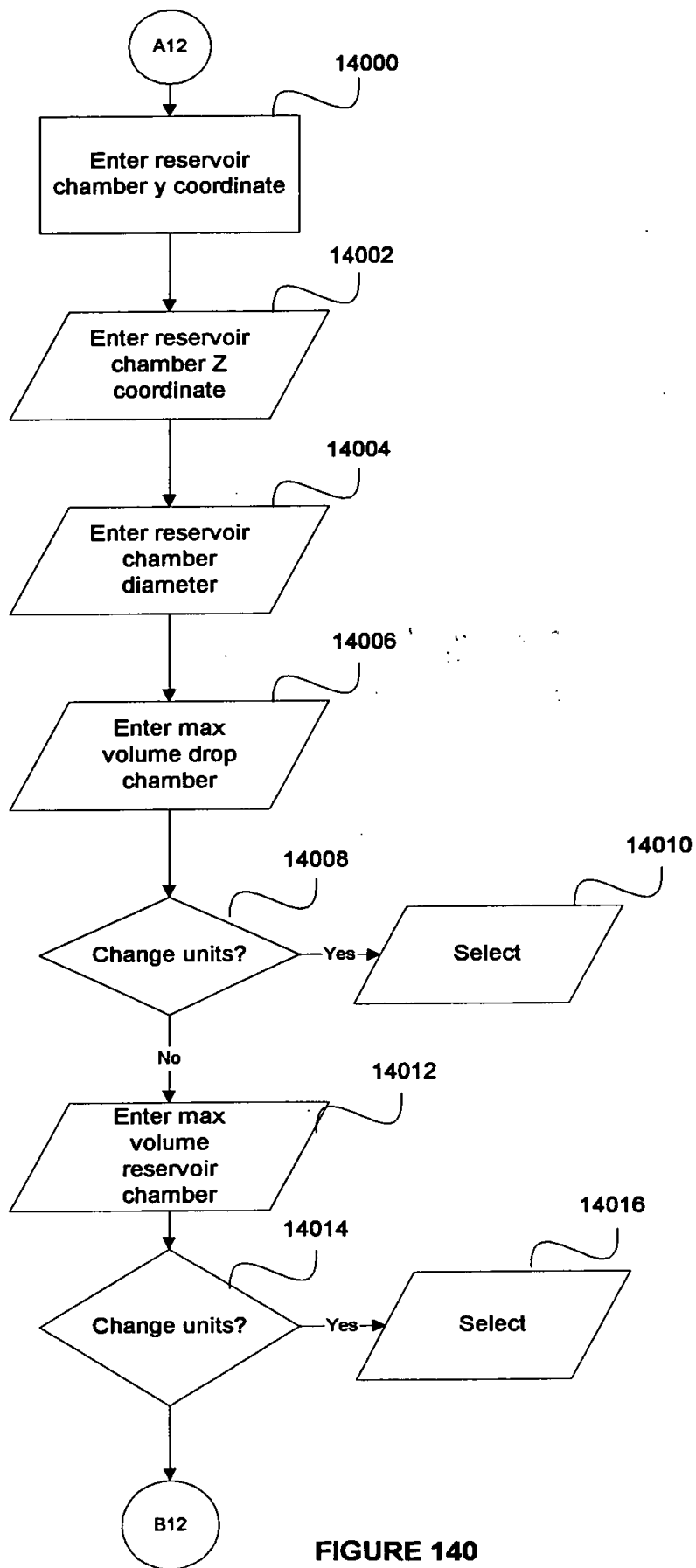


FIGURE 140

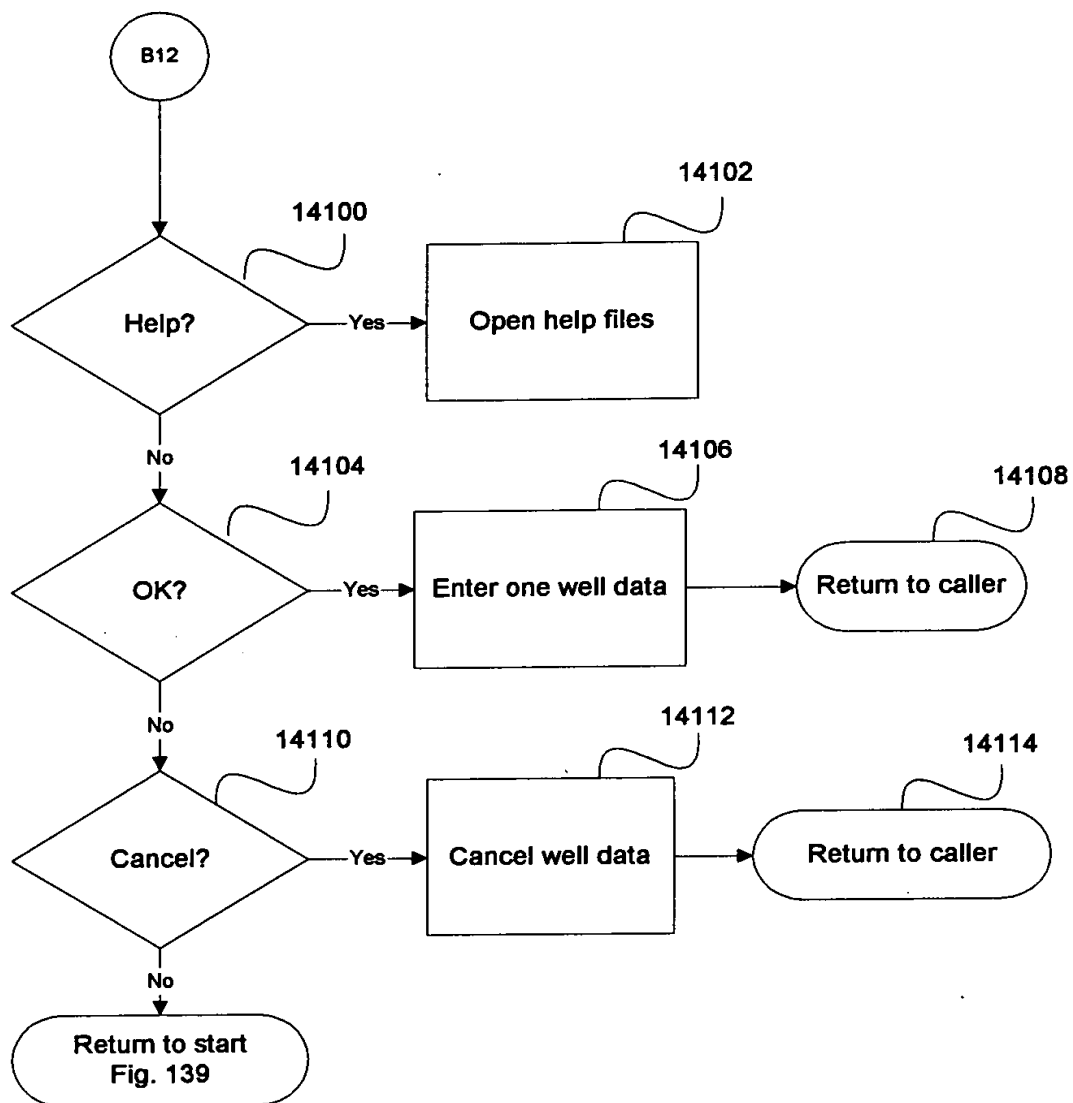


FIGURE 141

14201 14204 14200

### Autofill Apparatus Coordinates

Chamber coordinates in millimeter

	Drop	Reservoir
(1)	15	20
(2)	5	10
(3)	5	20
(4)	15	15
(5)	15	15
Diam.	5	10

14202 14206

Max Chamber Volume

Drop: 30  $\mu$ l ☒ 14212

Reservoir: 1000  $\mu$ l ☒ 14210

14208 14214 14216

Hint 14218

Autofill helps reducing to enter all the coordinates to fully describe a plate. It assumes that the plate has symmetric attributes, so that the above coordinates describe the plate uniquely.

You can overwrite coordinates afterwards by double clicking on a well.

Help... 14220

OK 14222

Cancel 14224

Fig.142

002080-587E960

New Apparatus

General apparatus data

Apparatus well data

AutoFill...

1

x

y

z

Drop: 15 5 5

Res: 20 10 20

Drop Diameter: 5

Res Diameter: 10

Max Vol Drop: 30.000  $\mu$ l

Max Vol Res:

2

x

y

z

Drop: 25 5 5

Res: 30 10 20

Drop Diameter: 5

Res Diameter: 10

Max Vol Drop: 30.000  $\mu$ l

Max Vol Res:

3

x

y

z

Drop: 35 5 5

Res: 40 10 20

Drop Diameter: 5

Res Diameter: 10

Max Vol Drop: 30.000  $\mu$ l

Max Vol Res:

4

x

y

Drop: 45 5

Res: 50 10

Drop Diameter: 5

Res Diameter: 10

Max Vol Drop: 30.0

Max Vol Res:

9

x

y

z

Drop: 15 15 5

Res: 20 20 20

Drop Diameter: 5

Res Diameter: 10

Max Vol Drop: 30.000  $\mu$ l

Max Vol Res:

10

x

y

z

Drop: 25 15 5

Res: 30 20 20

Drop Diameter: 5

Res Diameter: 10

Max Vol Drop: 30.000  $\mu$ l

Max Vol Res:

11

x

y

z

Drop: 35 15 5

Res: 40 20 20

Drop Diameter: 5

Res Diameter: 10

Max Vol Drop: 30.000  $\mu$ l

Max Vol Res:

12

x

y

Drop: 45 15

Res: 50 20

Drop Diameter: 5

Res Diameter: 10

Max Vol Drop: 30.0

Max Vol Res:

17

x

y

z

Drop: 15 25 5

Res: 20 25 20

Drop Diameter: 5

Res Diameter: 10

Max Vol Drop: 30.000  $\mu$ l

Max Vol Res:

18

x

y

z

Drop: 25 25 5

Res: 30 25 20

Drop Diameter: 5

Res Diameter: 10

Max Vol Drop: 30.000  $\mu$ l

Max Vol Res:

19

x

y

z

Drop: 35 25 5

Res: 40 25 20

Drop Diameter: 5

Res Diameter: 10

Max Vol Drop: 30.000  $\mu$ l

Max Vol Res:

20

x

y

Drop: 45 25

Res: 50 25

Drop Diameter: 5

Res Diameter: 10

Max Vol Drop: 30.0

Max Vol Res:

OK

Cancel

Help...

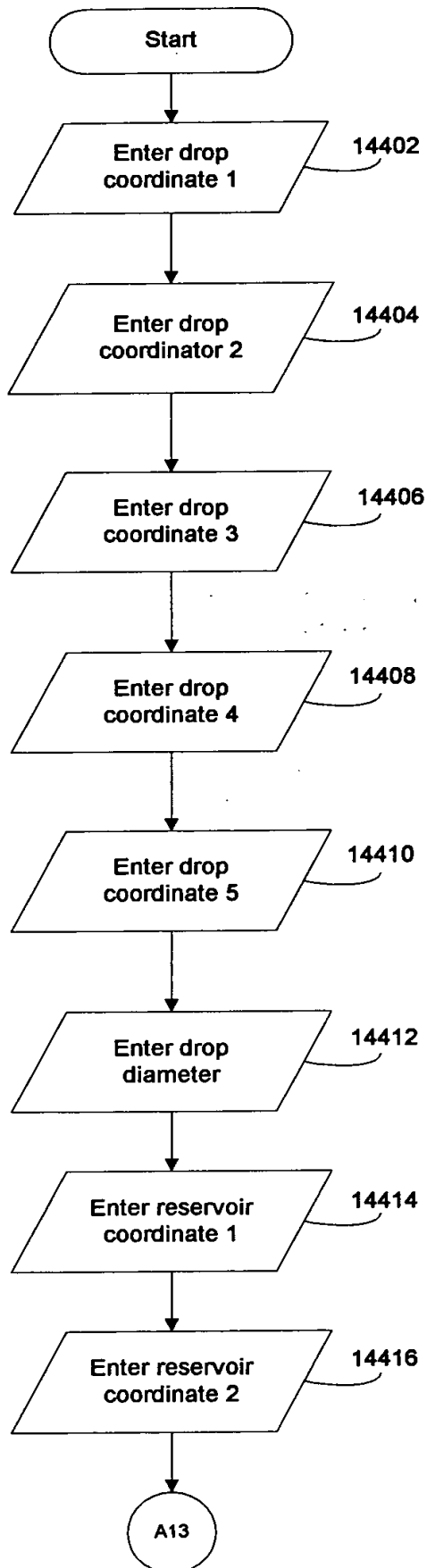
14300

14302

14304

Fig. 143

79



**FIGURE 144**

002000" 58T1E950

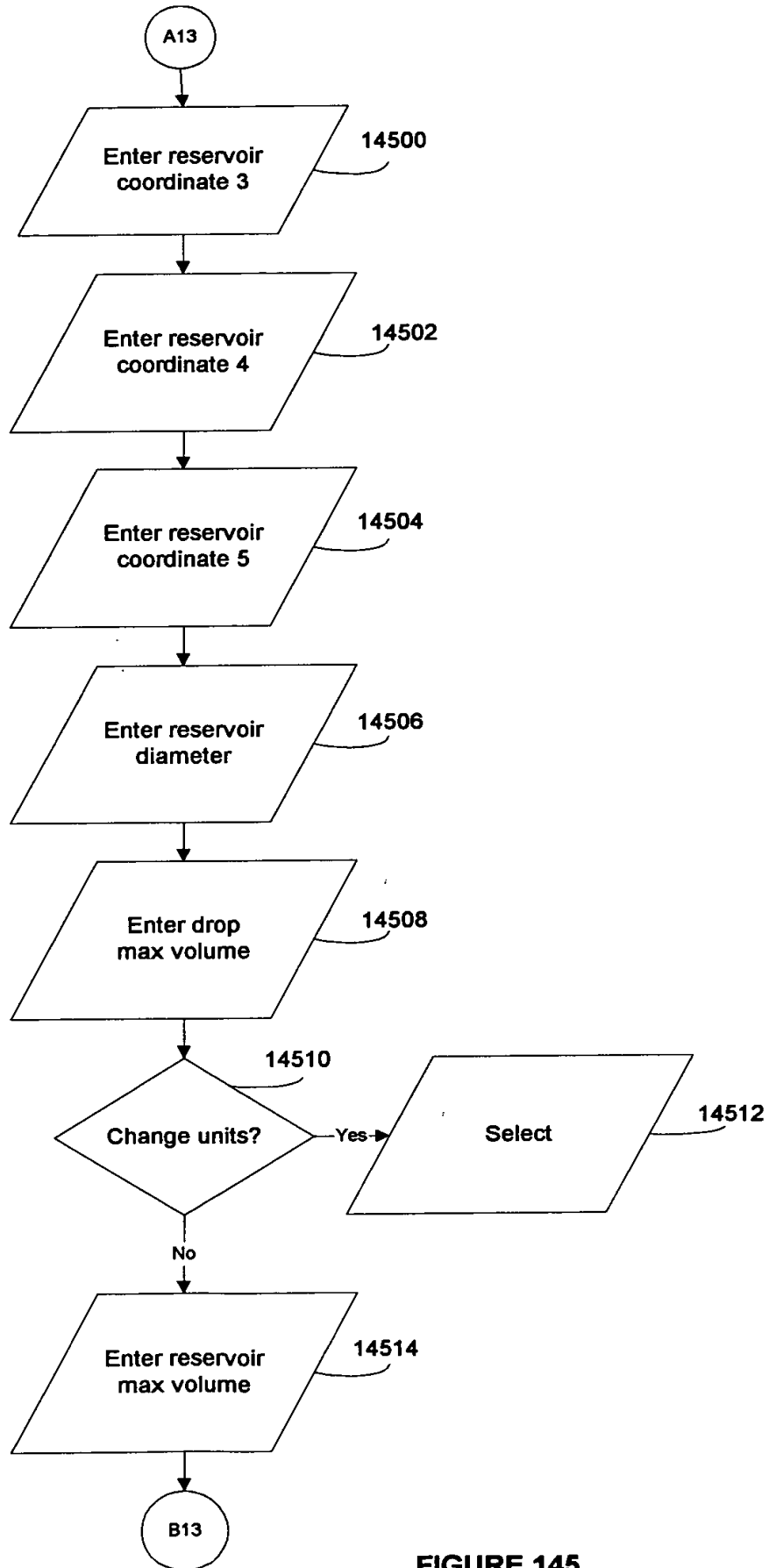


FIGURE 145

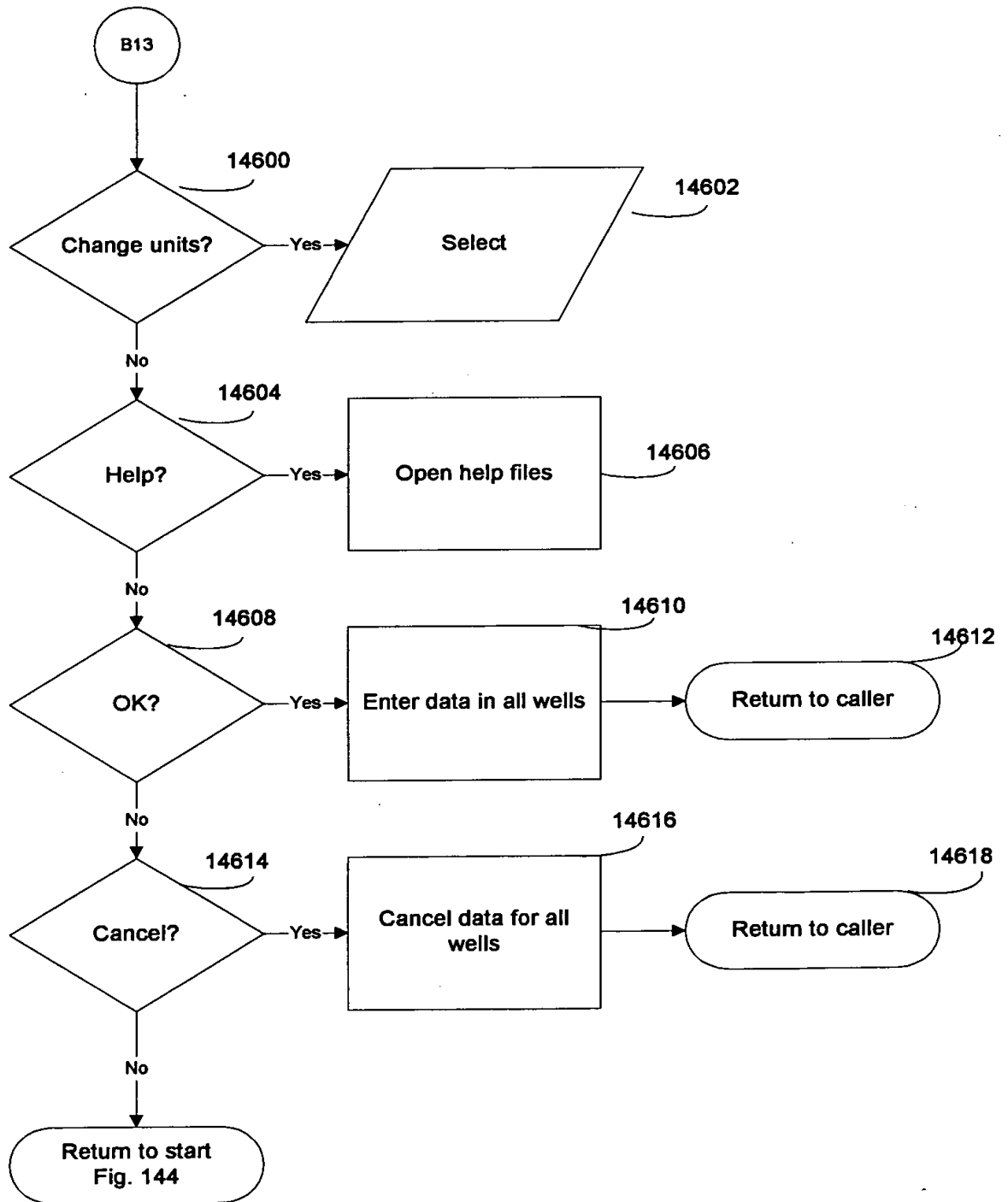


FIGURE 146

002030 5135 030200

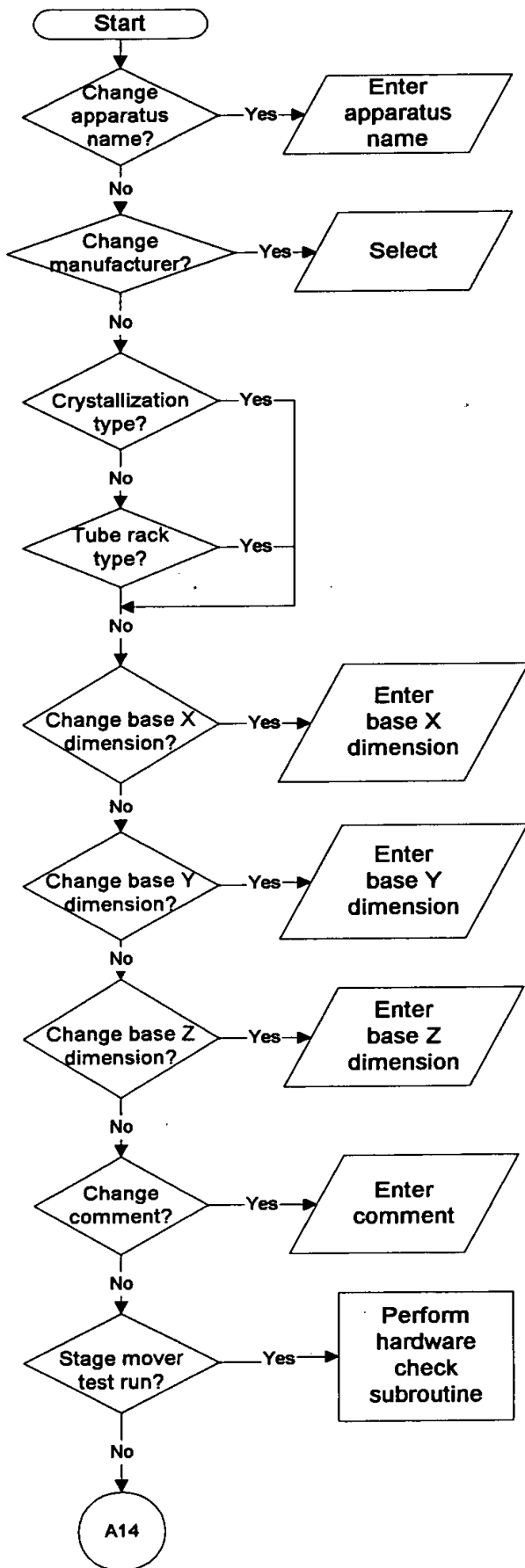


FIGURE 147



002020" 58T.E.950

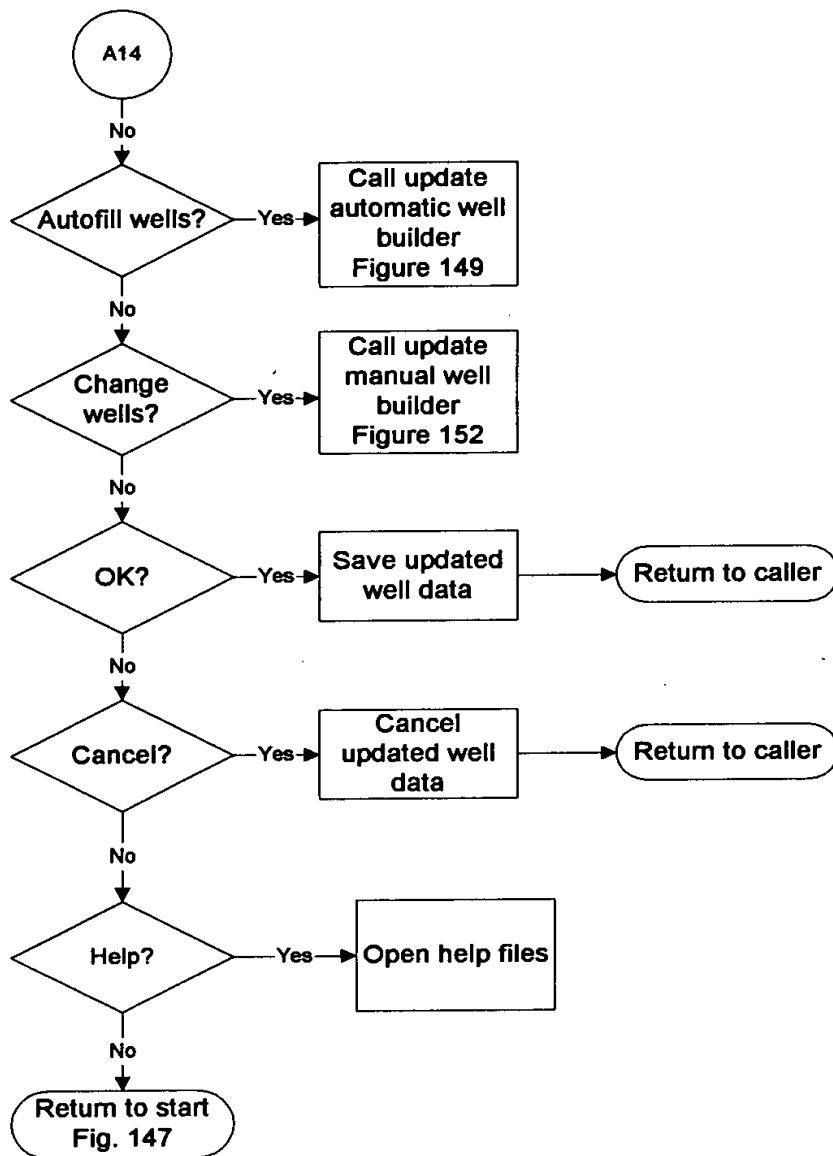


FIGURE 148

002080" 59TTE960

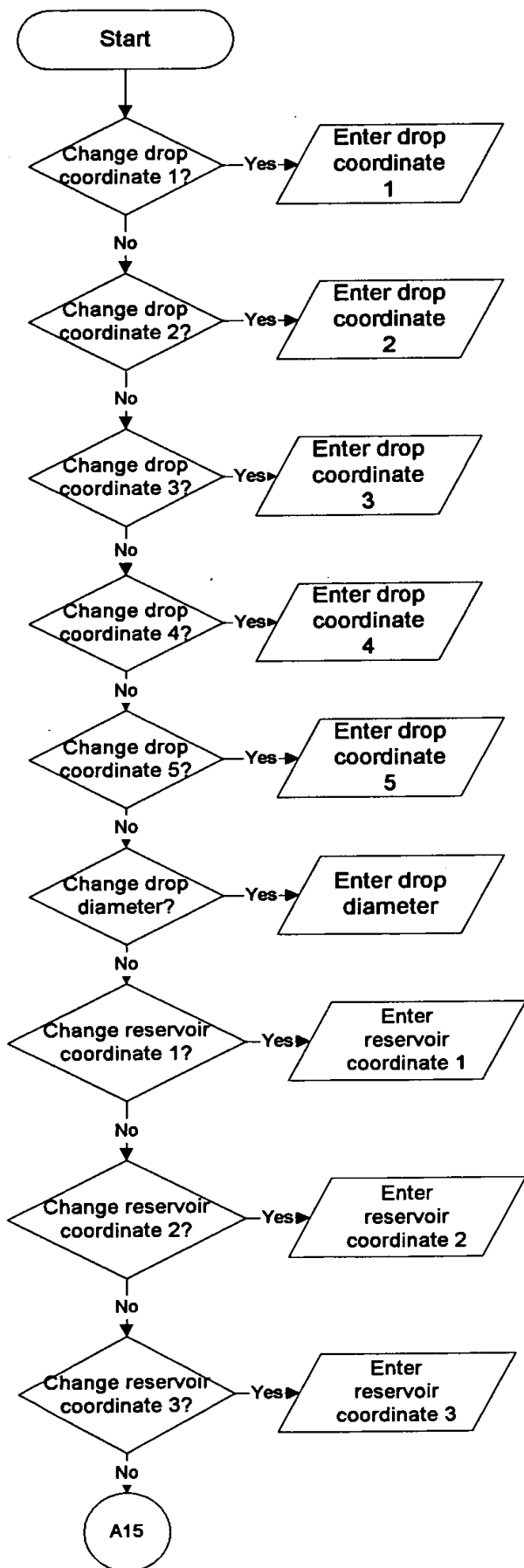


FIGURE 149

09631185.080200

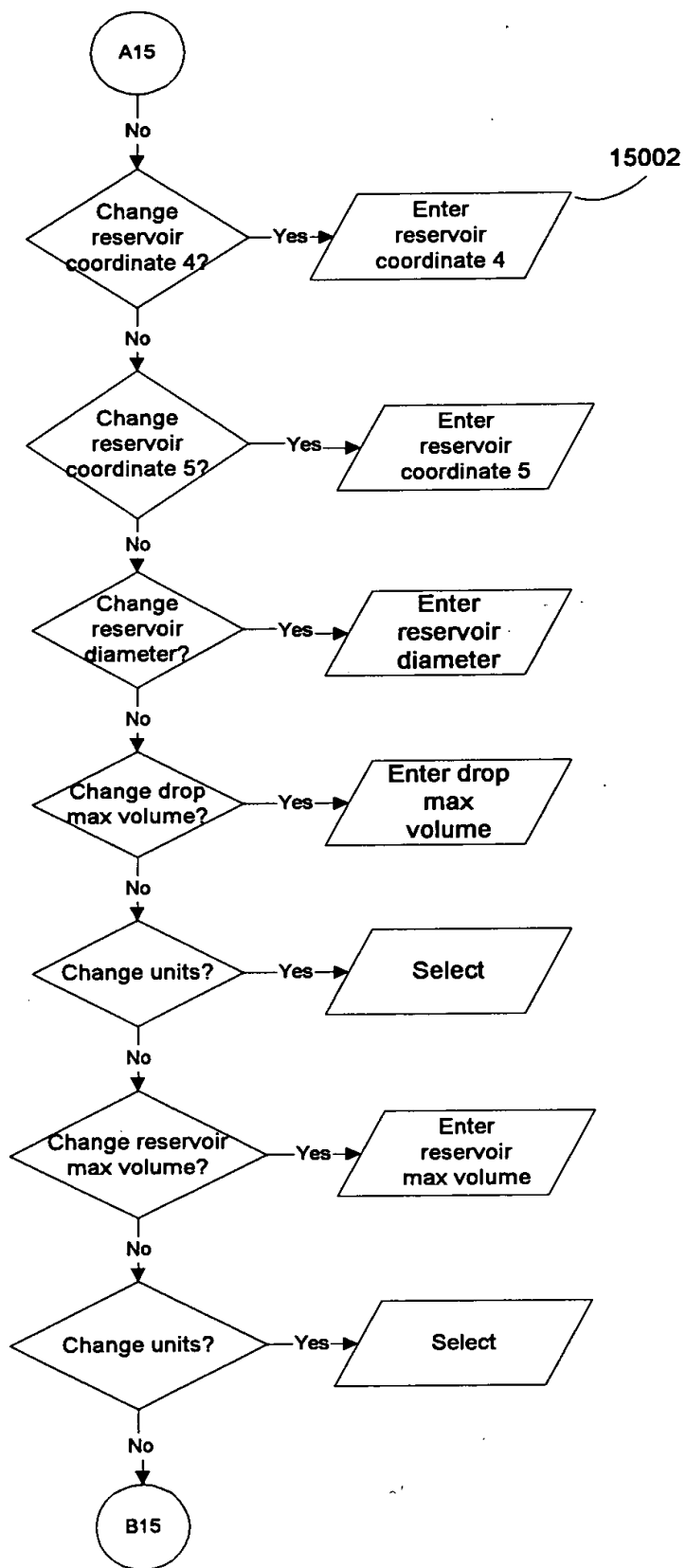


FIGURE 150

09631185-030200

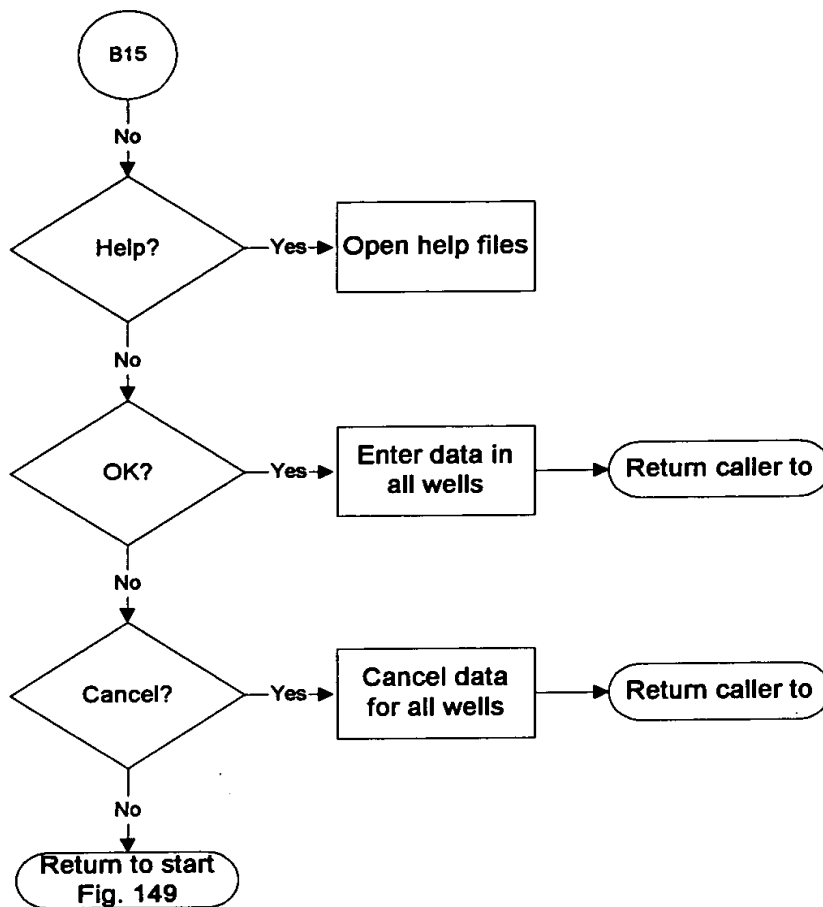


FIGURE 151

002080" ESTE 960

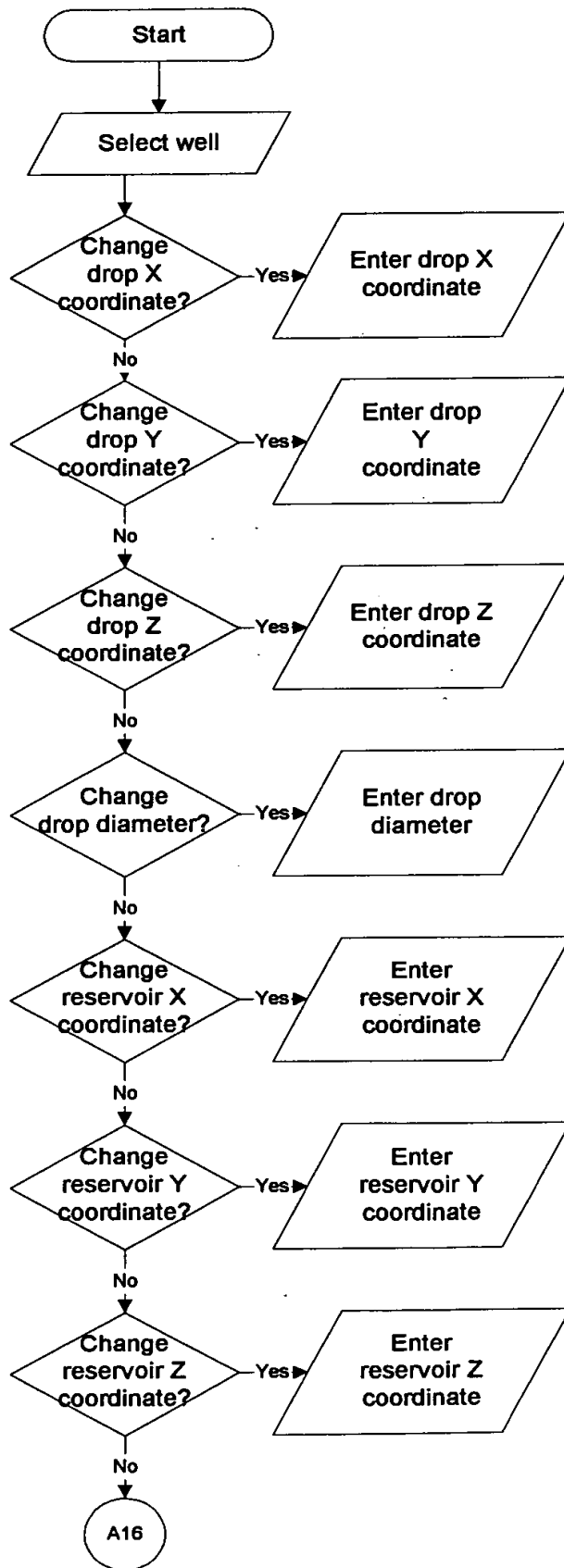


FIGURE 152

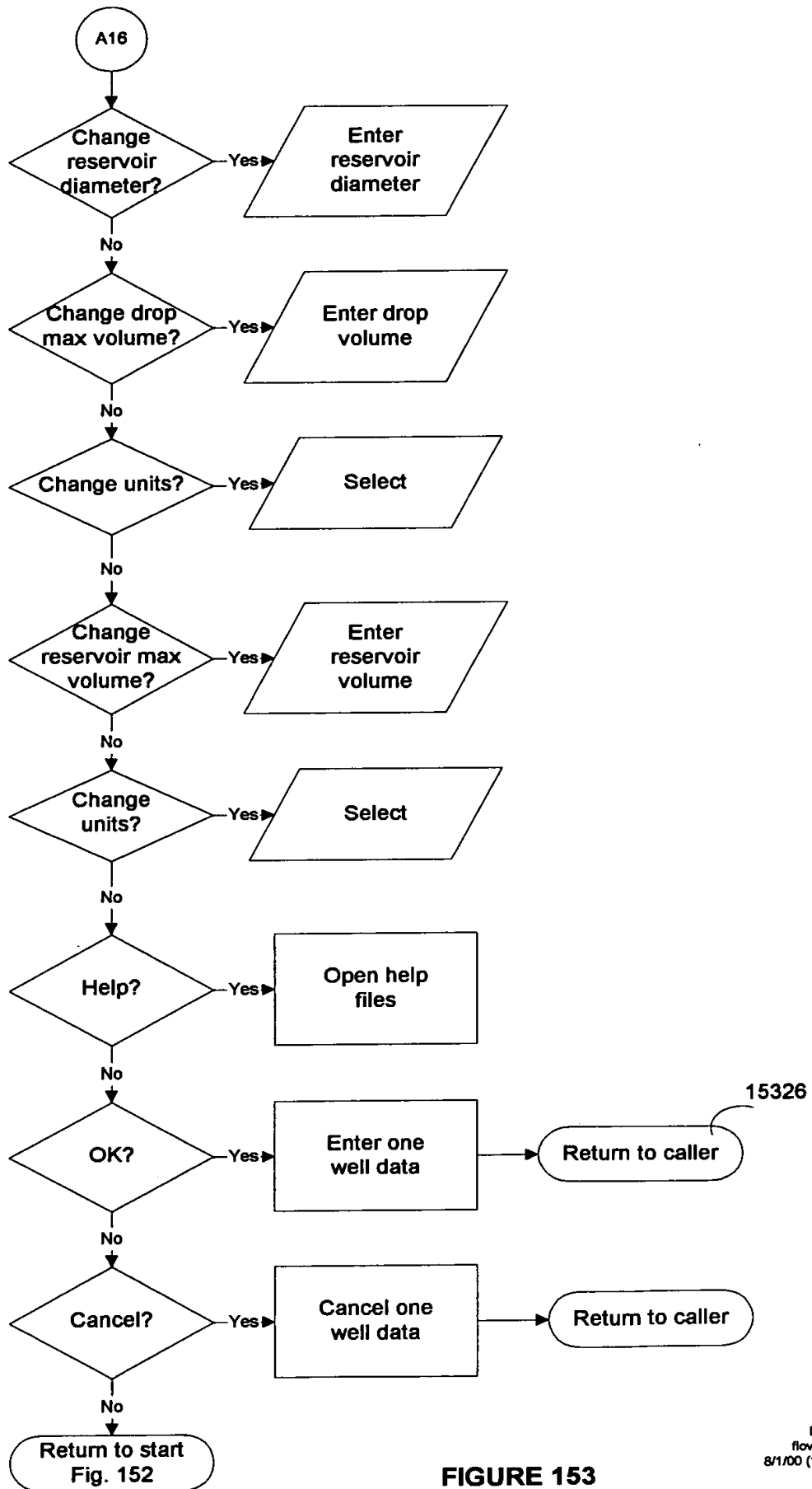


FIGURE 153

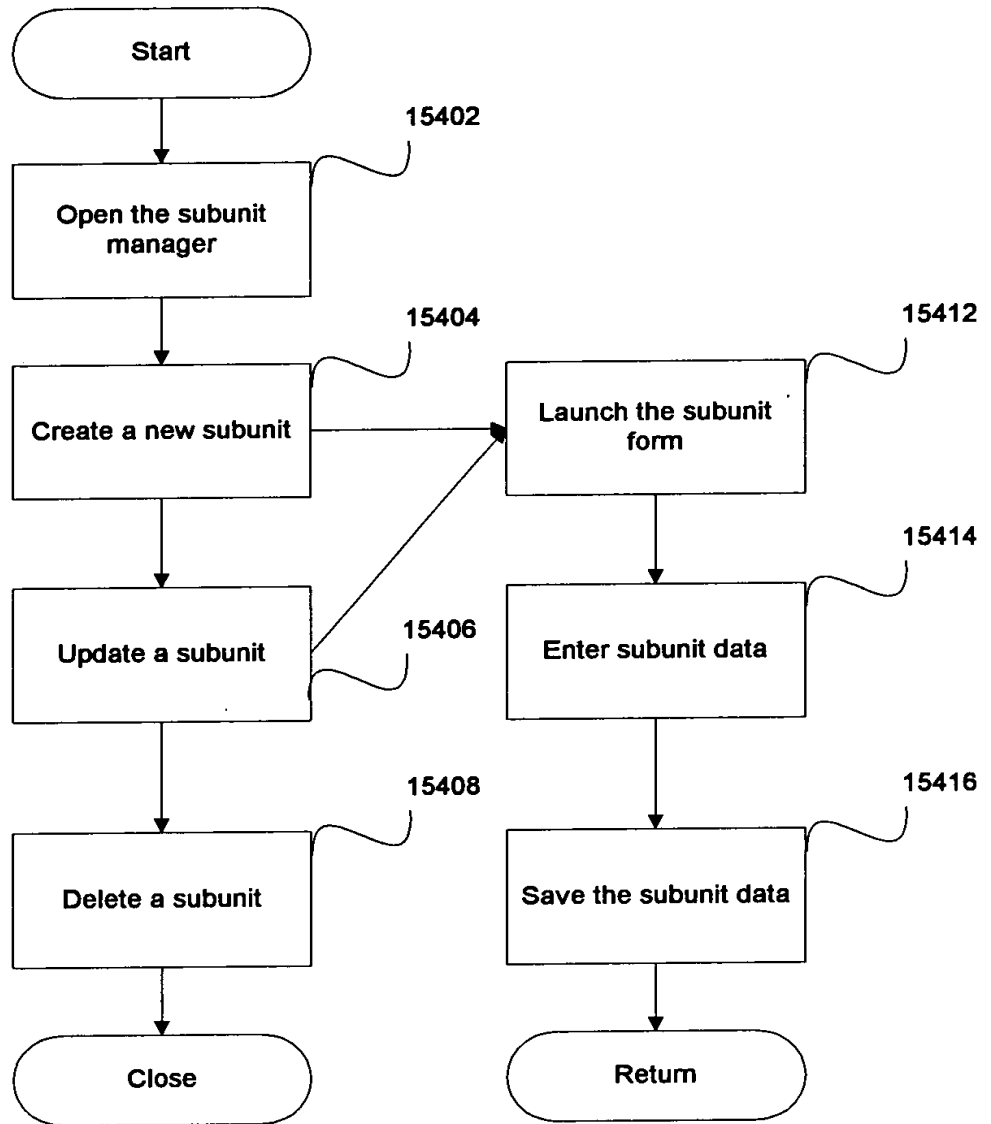


FIGURE 154

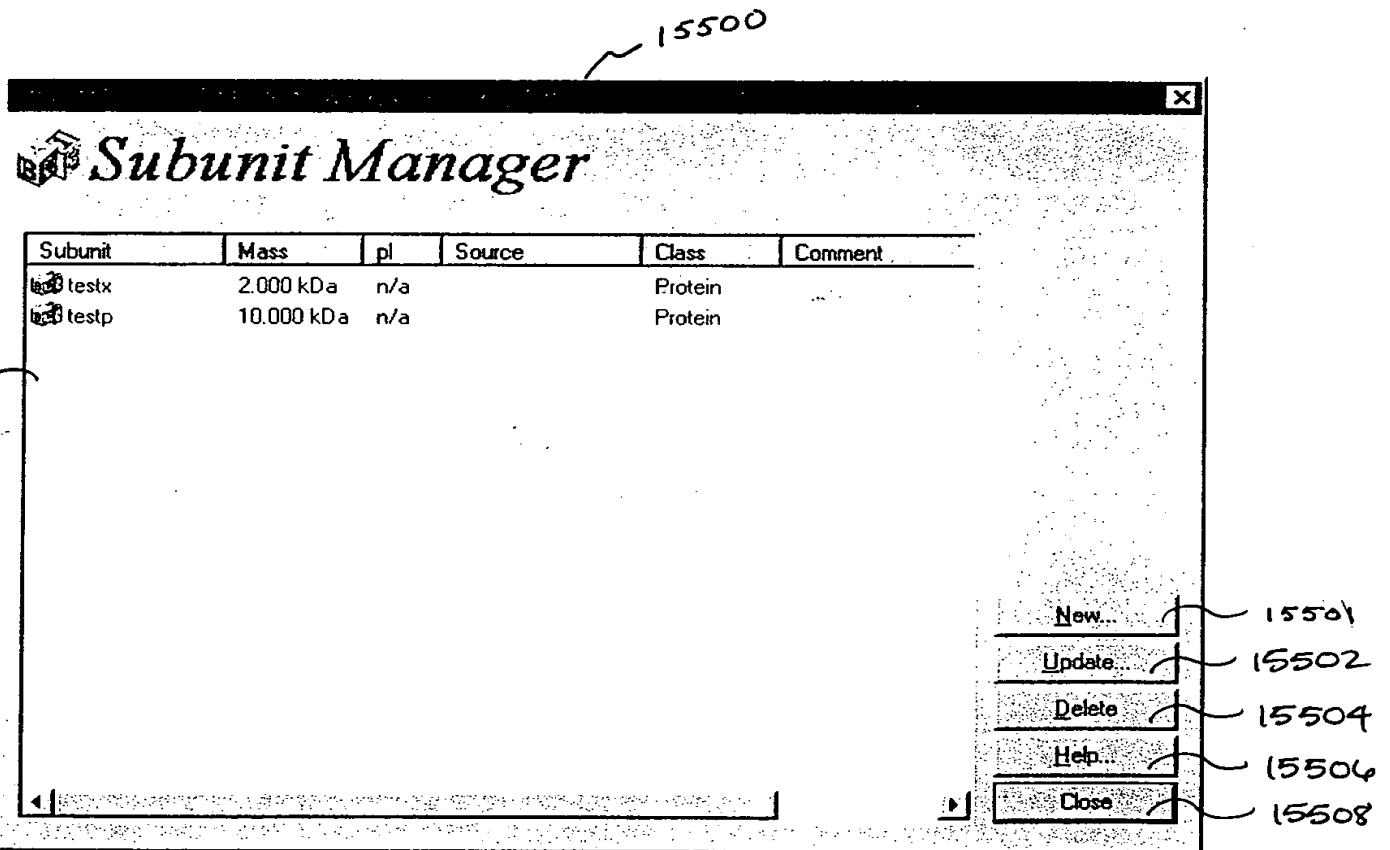
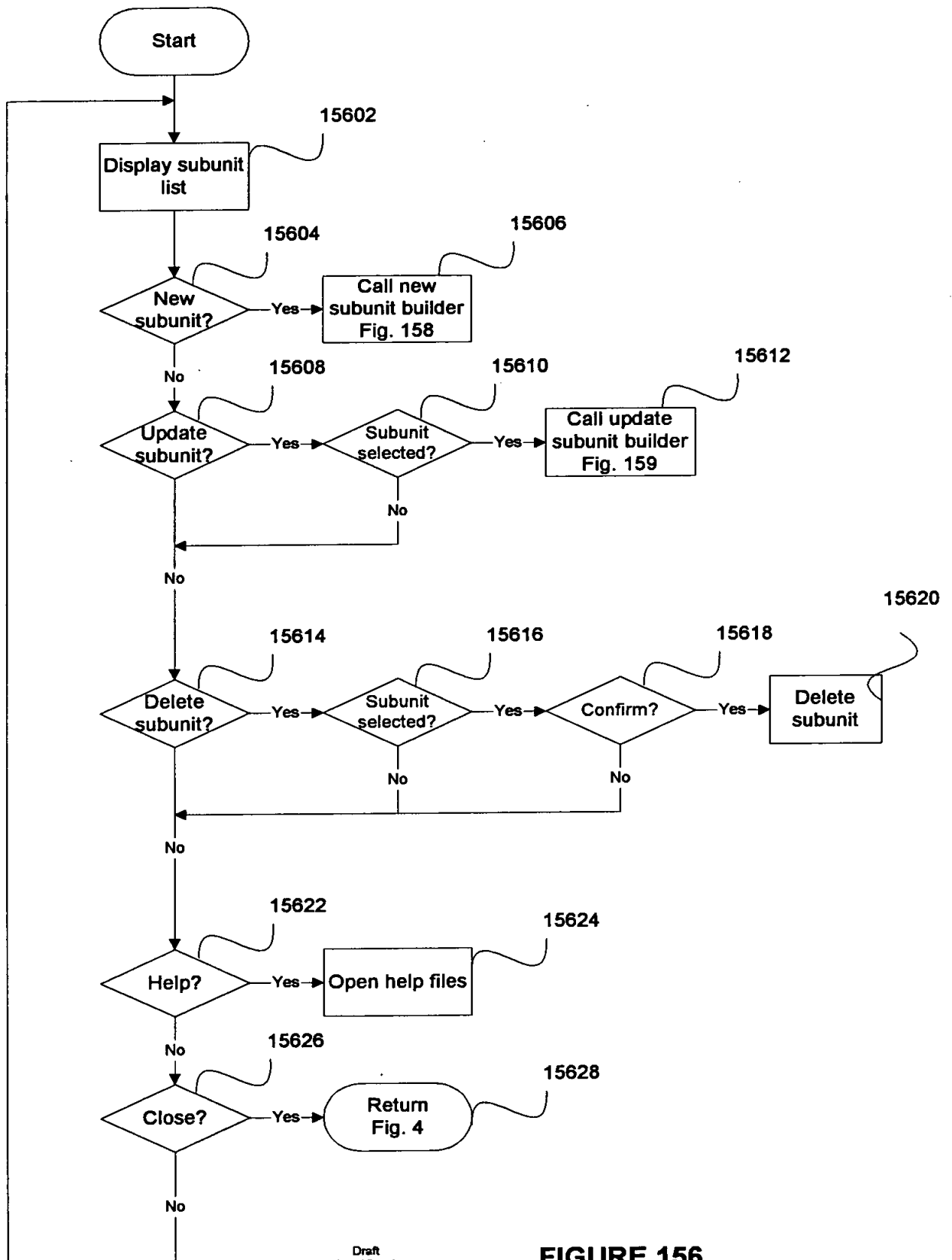


FIG. 155





002080" 58TTE960

15700

New Subunit

Attributes

Name: TbGAPDH 15701

Source: Trypanosoma brucei 15702

Class Name: Protein 15706

Mass: 40 kDa 15710

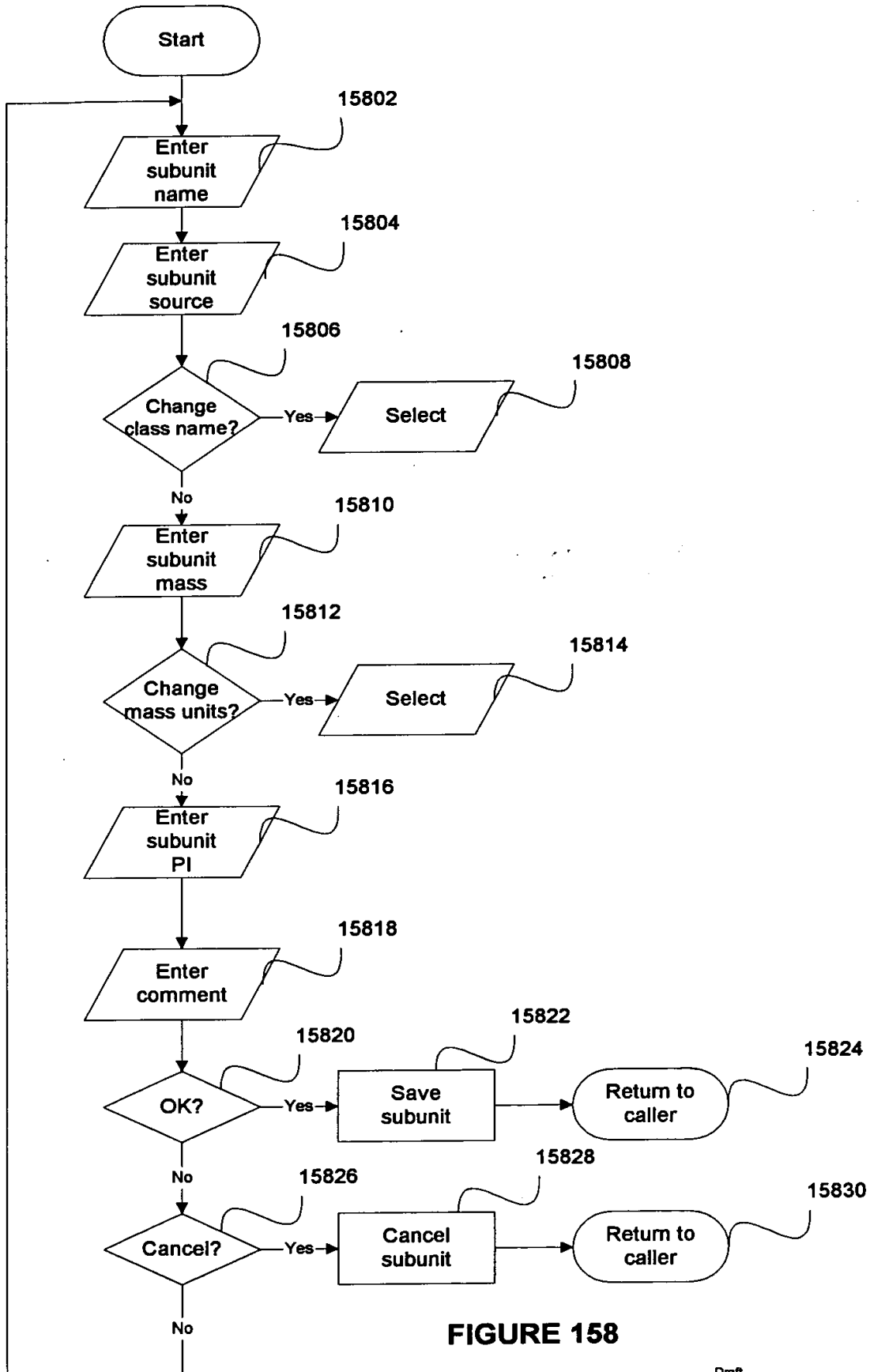
pI: 15712

Comment: 15714

Trypanosoma brucei  
glyceraldehyde-3-phosphate  
dehydrogenase 15716

OK 15718 Cancel 15720

Fig. 157



**FIGURE 158**

002030 " 58T 1:960

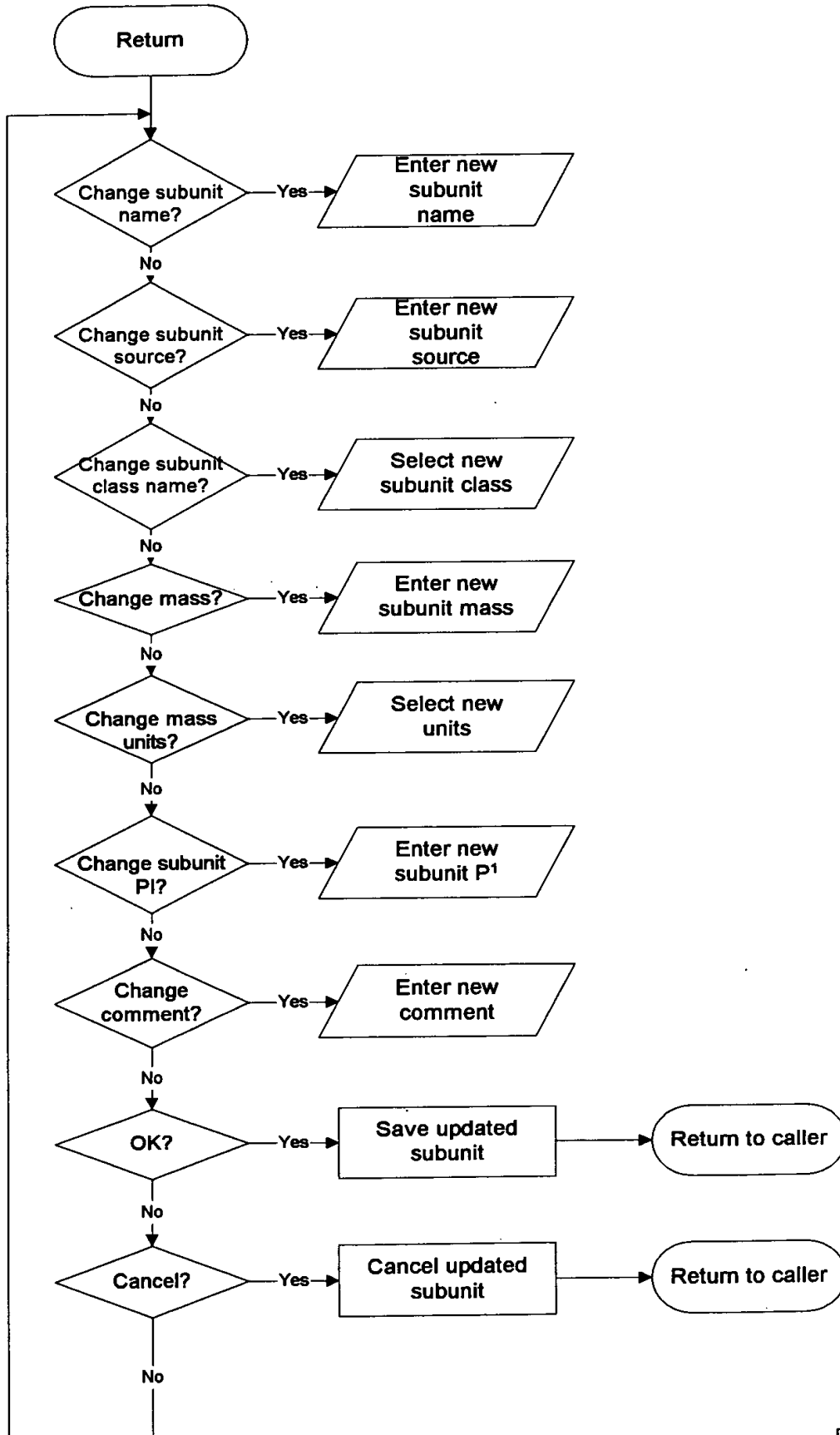
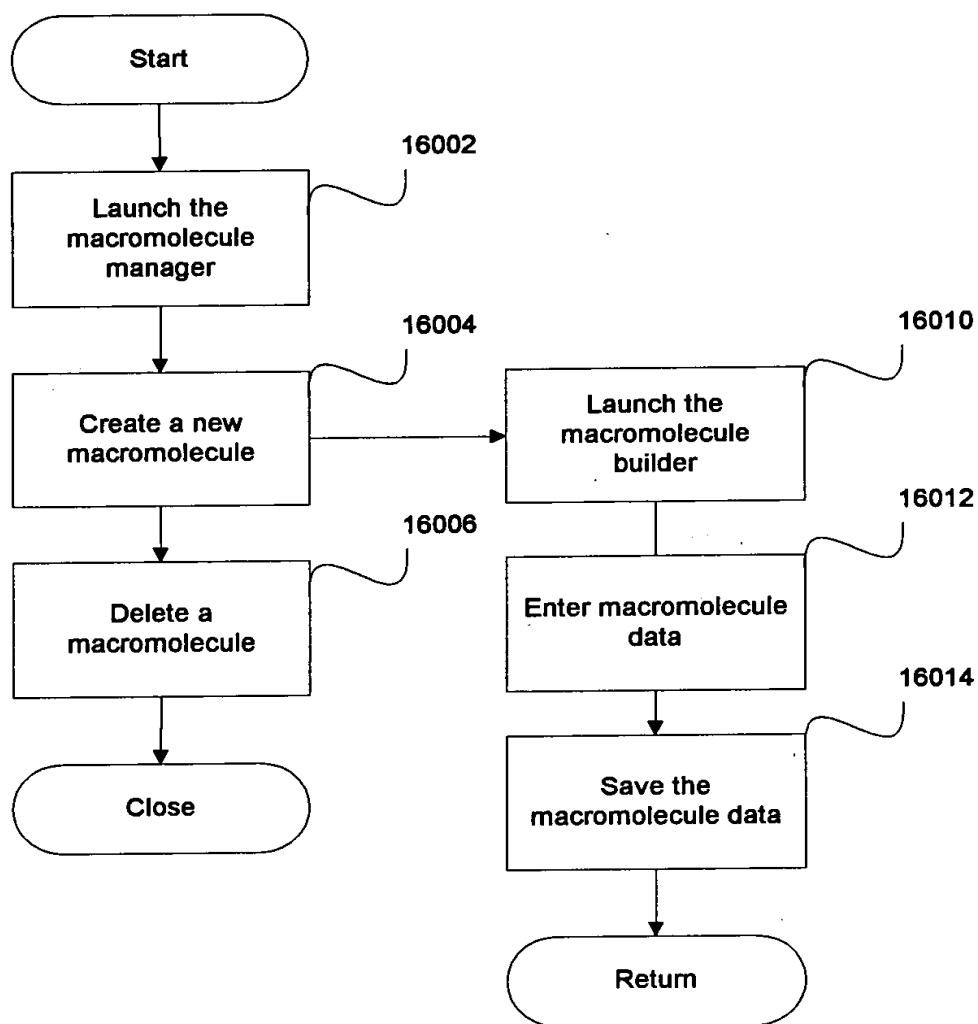


FIGURE 159



**FIGURE 160**

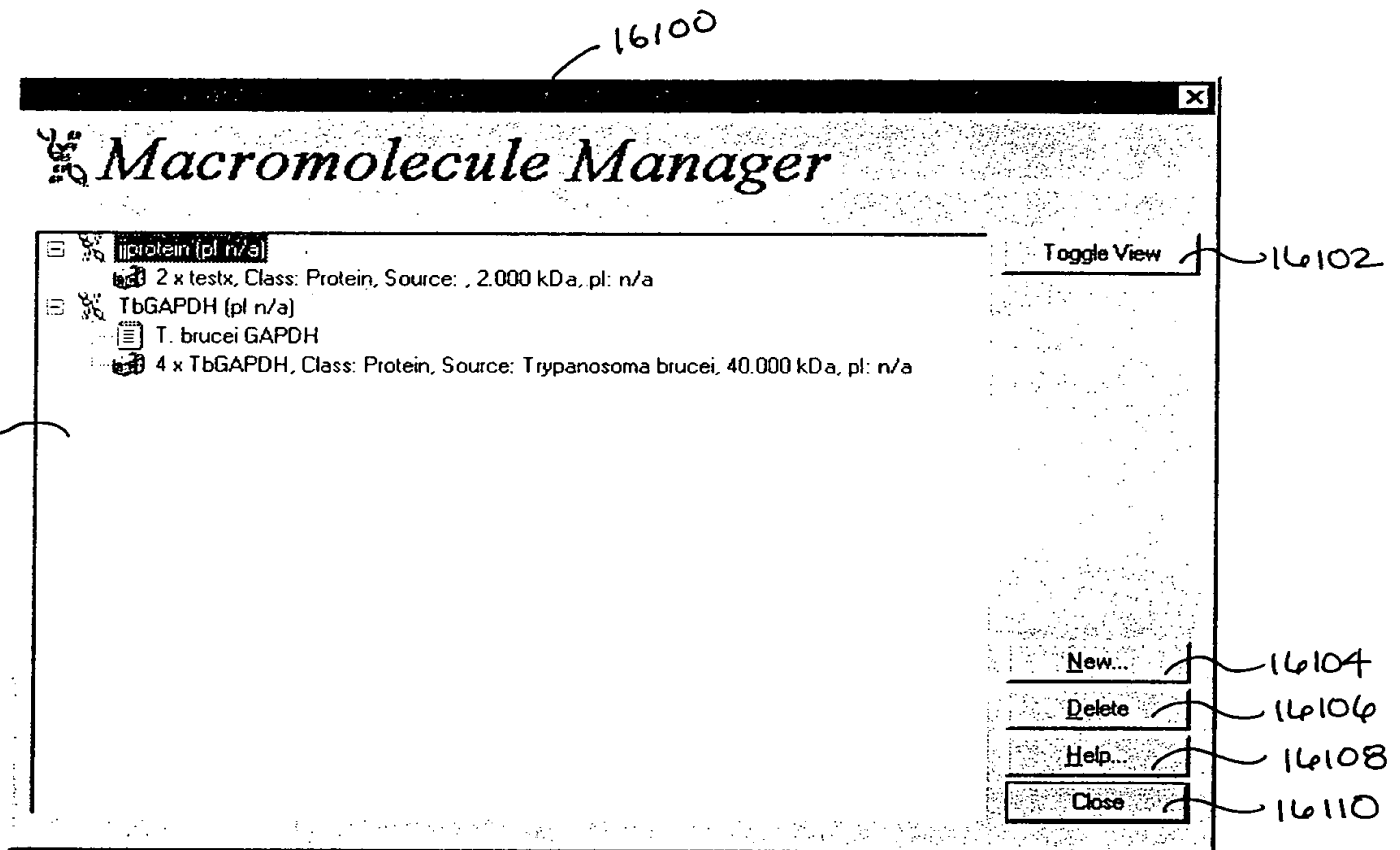
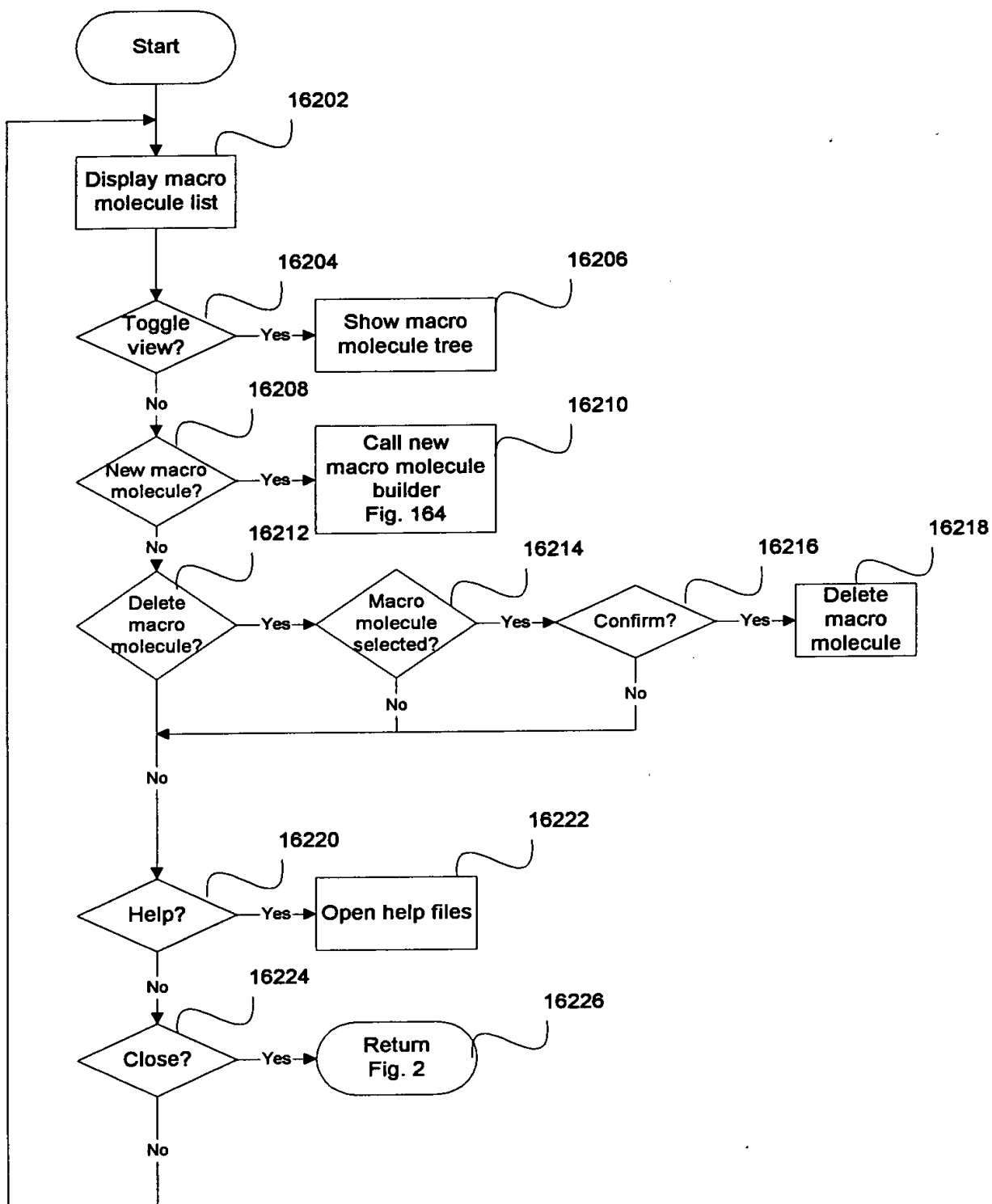


FIG. 161



16300

16304

16301

16302

Macromolecule Builder

Subunits: Create Subunit...

Subunit	Mass	pI	Source
testx	2.000 kDa	n/a	
testp	10.000 kDa	n/a	
TbGAPDH	40.000 kDa	n/a	Trypar

Molecule Name: 4testx

pI:

Molecule Class: Protein

Comment: testx holo-tetramer

Subunits associated with new Molecule:

Count	Subunit	Mass	pI	Source
4	testx	2.000 k...	n/a	

16312

16314

16316

16318

16320

16306

16308

16310

Cancel

Help...

Fig. 163



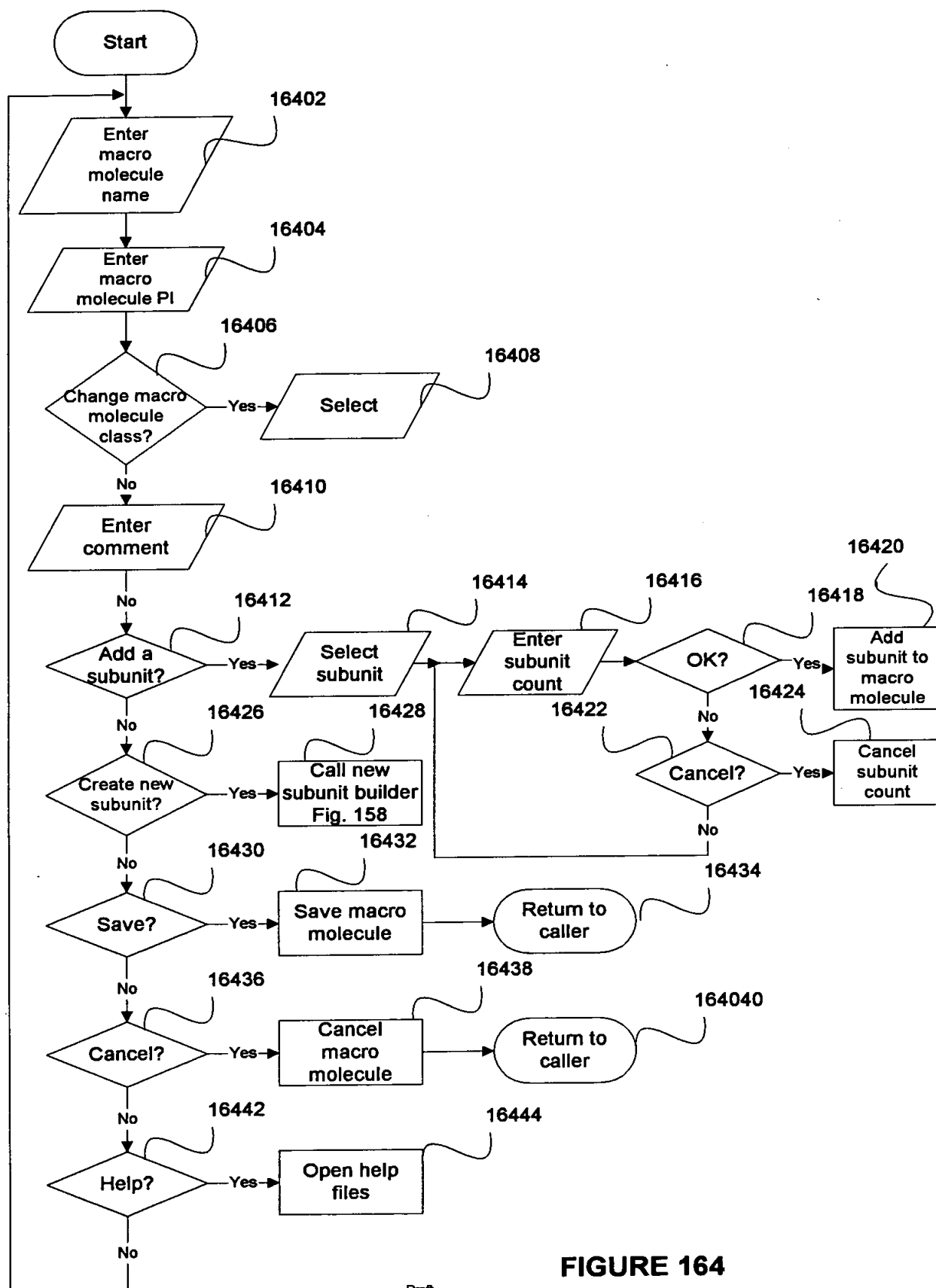
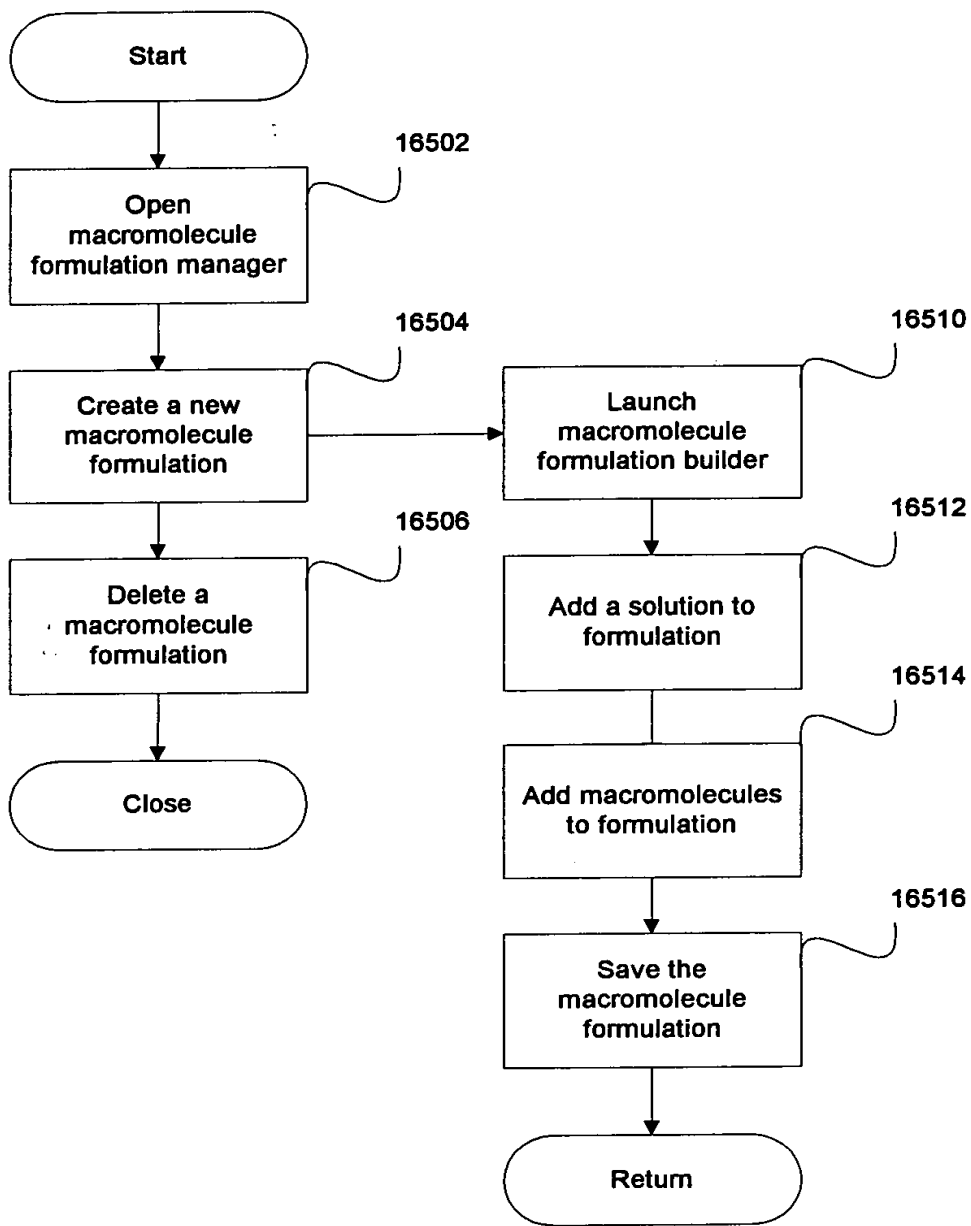


















FIGURE 164



**FIGURE 165**



  **ii**protein040300  
 Conduct: n/a; Osmol: n/a; Visco: Low; Final pH: n/a  
 ChangeTracking.txt  
 Admin (Mon, Apr 03 2000 11:25 AM)  
 H2O (H2O)  
 150.000 mM sodium chloride (Sigma Chemical Co. S7653)  
 10.000 mg/ml ii**protein** (pl: n/a)  
  **ii**protein040300b  
  **ii**protein040500  
 Conduct: n/a; Osmol: n/a; Visco: Low; Final pH: n/a  
 15 mg/ml ii**protein** in saline  
 ii**protein**purification.doc  
 Admin (Wed, Apr 05 2000 03:29 PM)

**New..**

**New..**

Delete...

Delete...

**Help...**

**Help...**

Close

Close

**Usage:**

ProjectName	Comment
protein	
test	

Fig. 1466

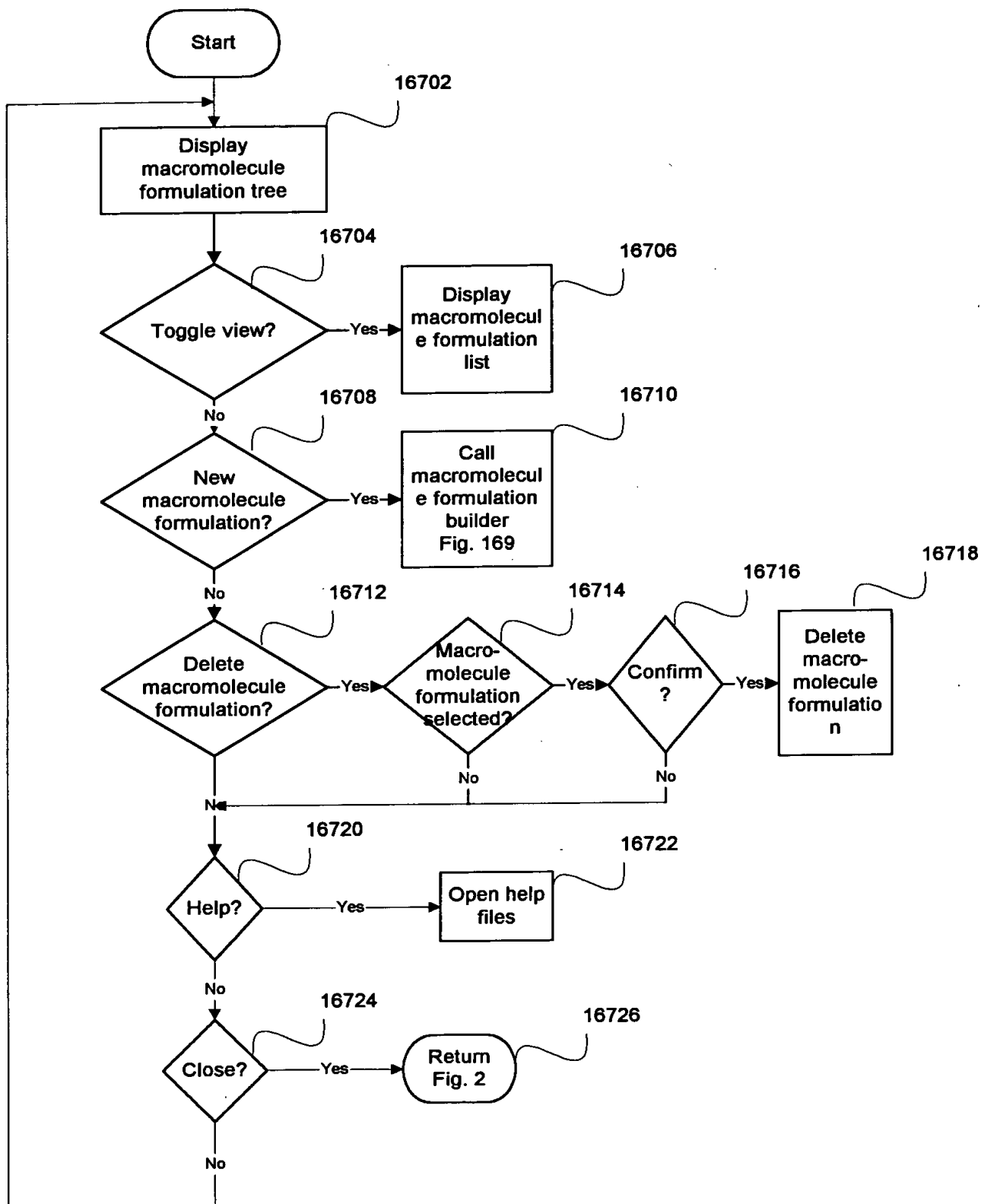


FIGURE 167

002080" 5811E500

Macromolecule Formulation Builder

Solutions | Macromolecules

New Macromolecule...

16802

16808

16800

16804

16814

16825

16806

16816

16801

16812

16810

16818

16822

16820

16824

16827

16826

16828

16830

Molecule List

15.000 mg/ml 4testx

Solution: saline

Prep. Date: 4/ 7/00

Storage Temp: 4 C

Preparator: Admin

Macromolecule Formulation Name: iiprotein040700

E:\crymon\Help\crystalmonitor\images\ijprot

Comment: 15 mg/ml iiprotein in saline

16826

16828

16830

FIG. 168

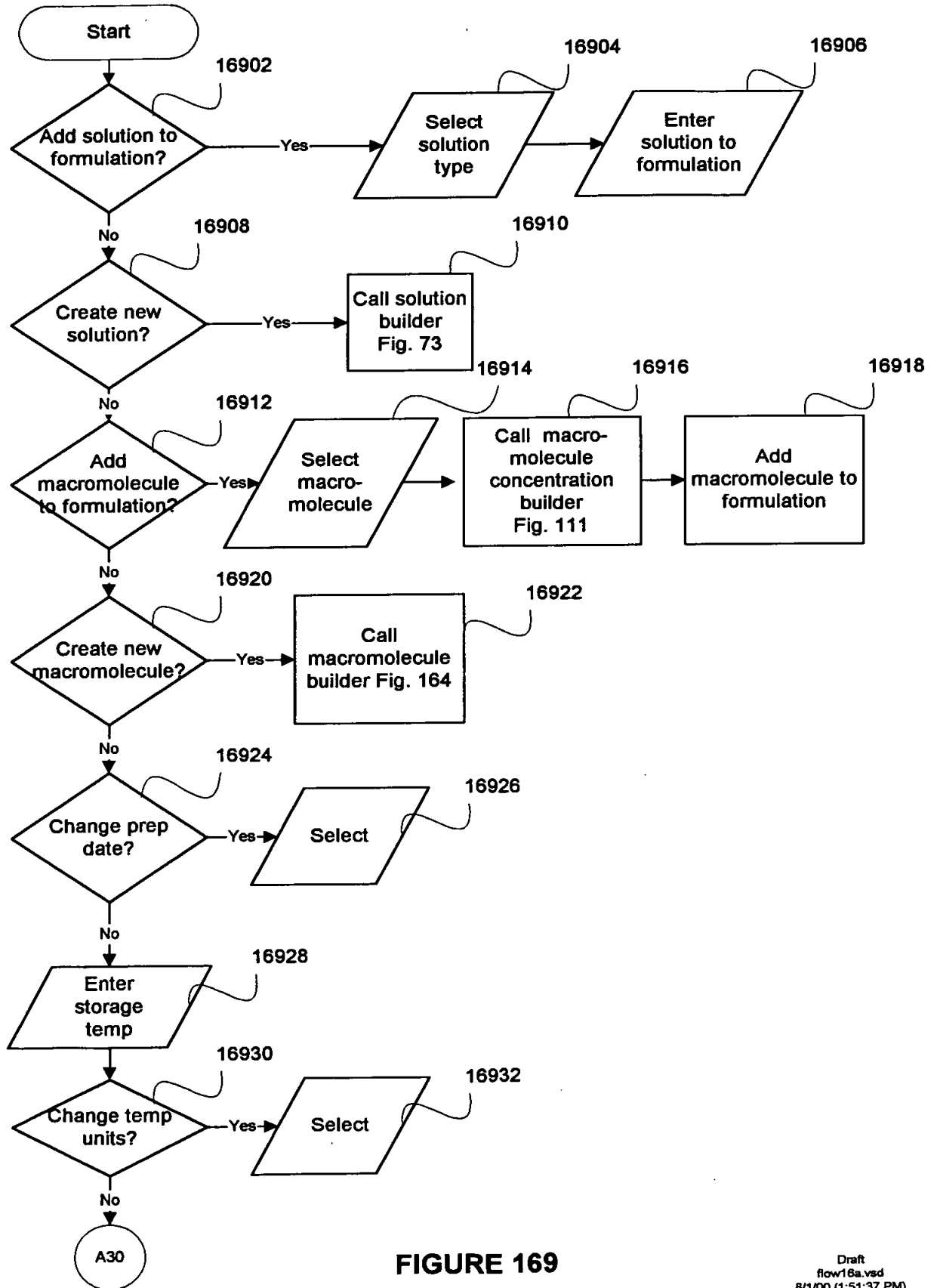


FIGURE 169

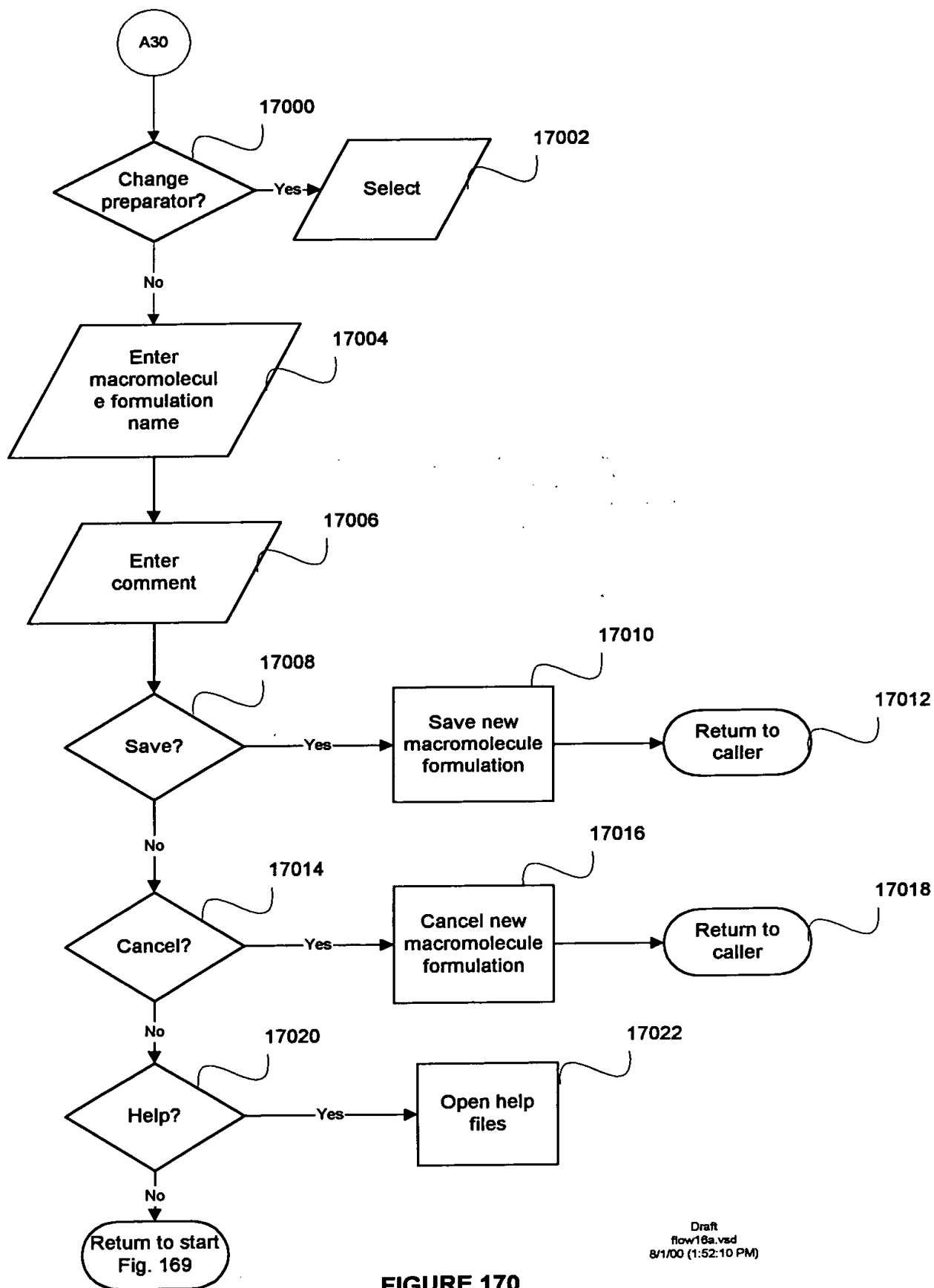


FIGURE 170

002080" 5877E360

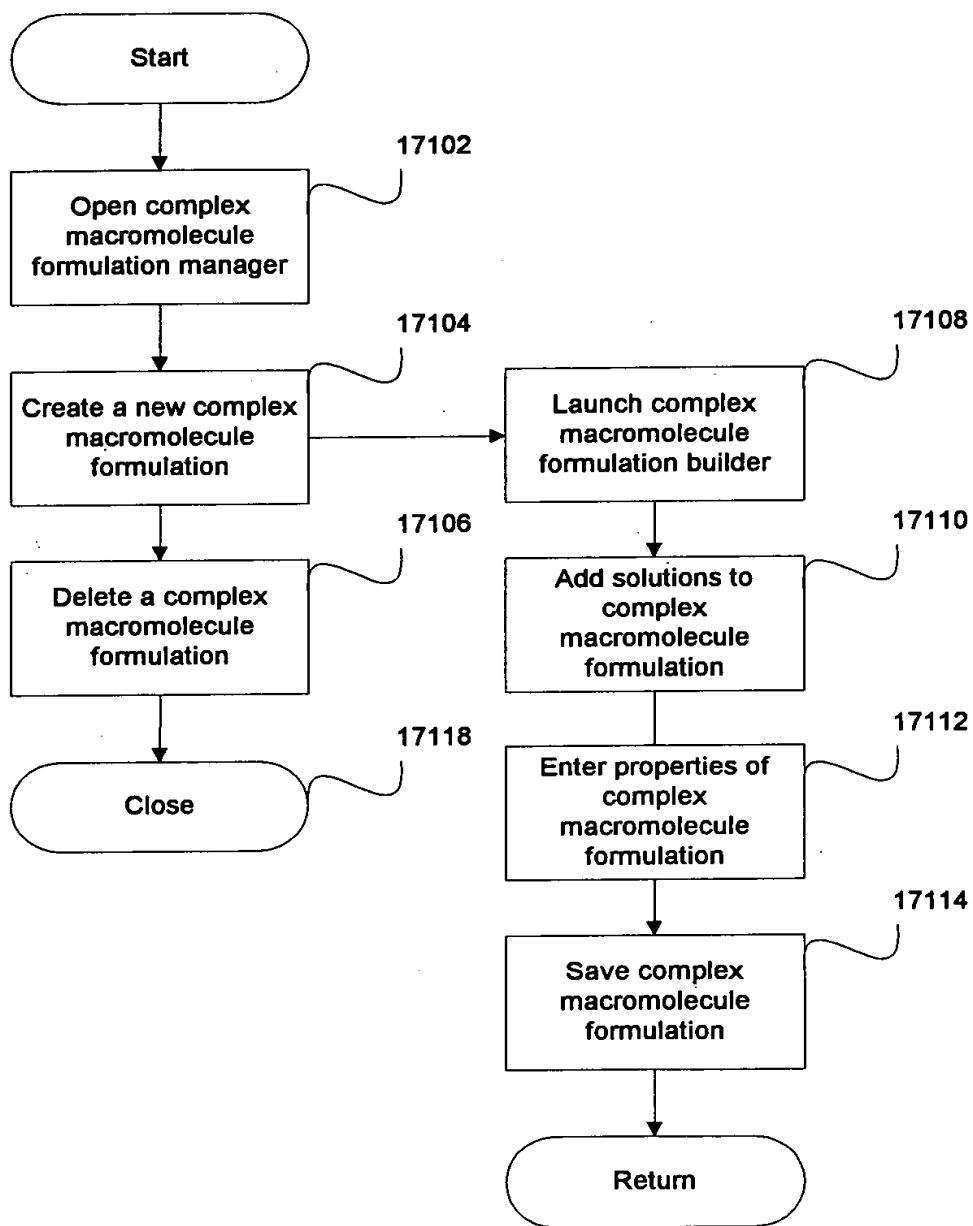


FIGURE 171





002090" 54T E960

17201

17200

### Complex Macromolecule Form. Mgr.

**dualjprotein040500**

- Conduct: n/a; Osmol: n/a; Visco: Low; Final pH: n/a
- Admin (Wed, Apr 05 2000 03:51 PM)
- H2O (H2O)
- 150.000 mM sodium chloride (Sigma Chemical Co. S7653)
- 12.500 mg/ml ijprotein (pl: n/a)
- newtest

Toggle View

New...

Delete...

Help...

Close

Usage:

ProjectName	Comment
ijprotein	

7204

17202

17206

17208

17210

17212

FIG. 172

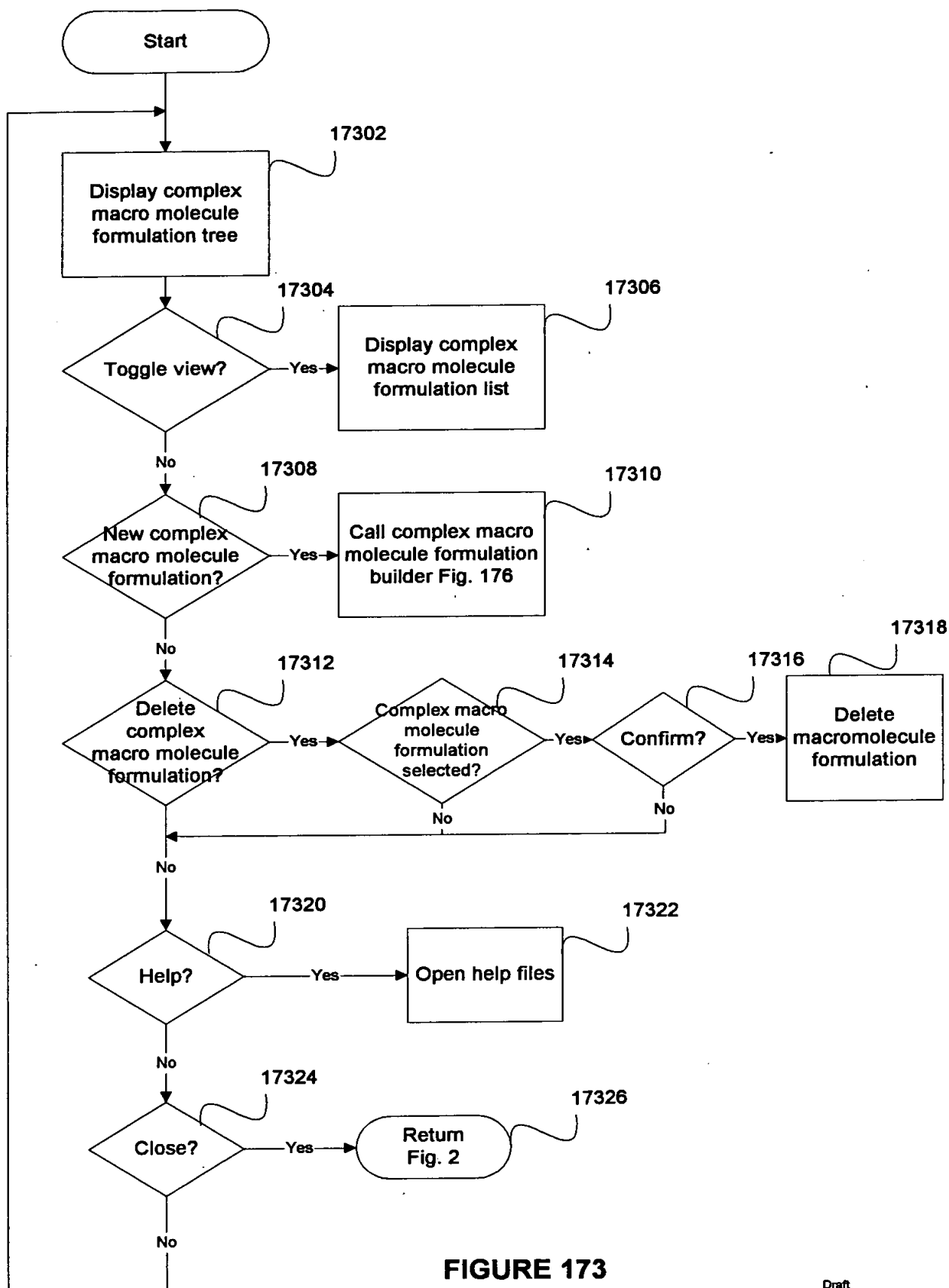


FIGURE 173

002080-58772960

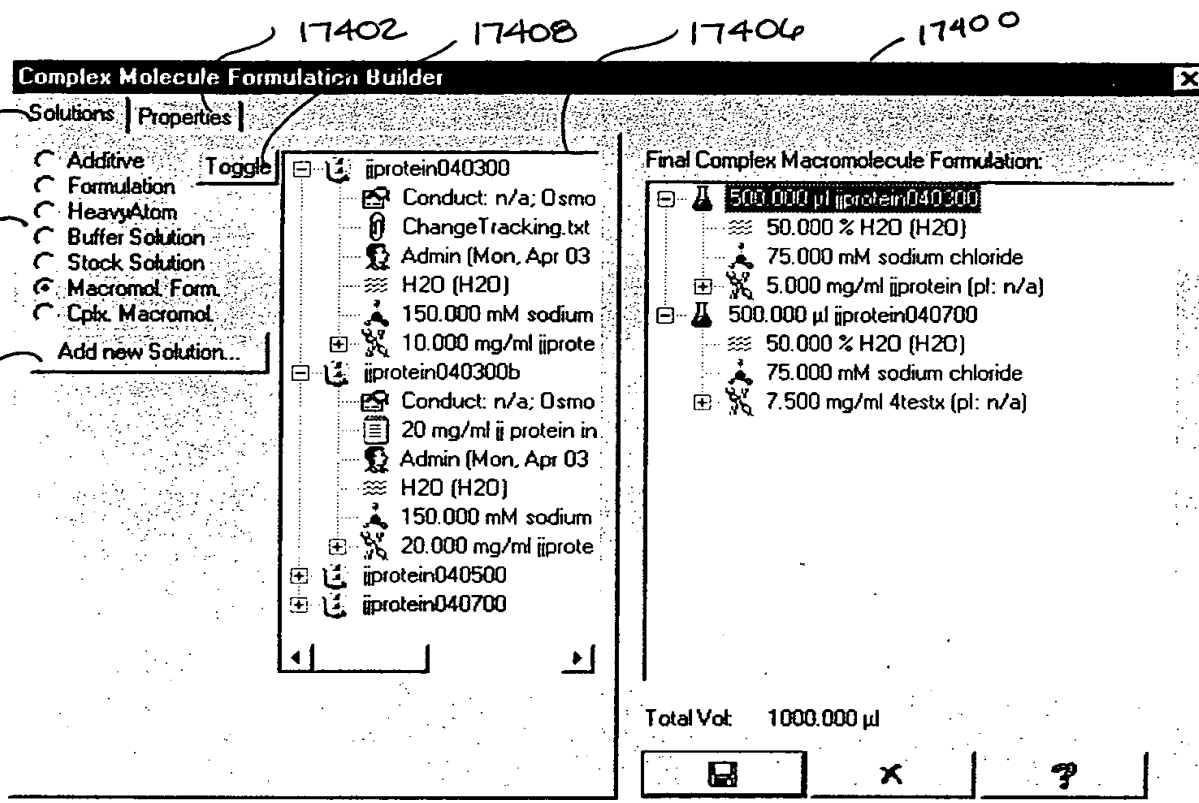


Fig. 174

003080" 551135.080200

17500 17530 17528 17508 17510 17512

**Complex Molecule Formulation Builder** [X]

Solutions | Properties

17501 Timestamp: 4/ 7/00

17502 Storage Temp: 4

17504 Preparator: Admin

17506 Final pH:

17506 Conductivity:  $\mu\text{S}/\text{cm}$

17520 Vapor Pressure Osmolality: mmole/kg

17522 Solvent: H2O (Mothe)

17524 New Solution Name: iiproteincomplex37

17524 Viscosity: Low High

17526 Comment: mix iiprotein040300 and iiprotein040700

17538

17536

**Final Complex Macromolecule Formulation:**

- 500.000  $\mu\text{l}$  iiprotein040300
- 50.000 % H2O (H2O)
- 75.000 mM sodium chloride
- 5.000 mg/ml iiprotein (pl: n/a)
- 500.000  $\mu\text{l}$  iiprotein040700
- 50.000 % H2O (H2O)
- 75.000 mM sodium chloride
- 7.500 mg/ml 4testx (pl: n/a)

17514

17516

17518

17534

Total Vol: 1000.000  $\mu\text{l}$

17540 X 17542 ? 17544

Fig. 175

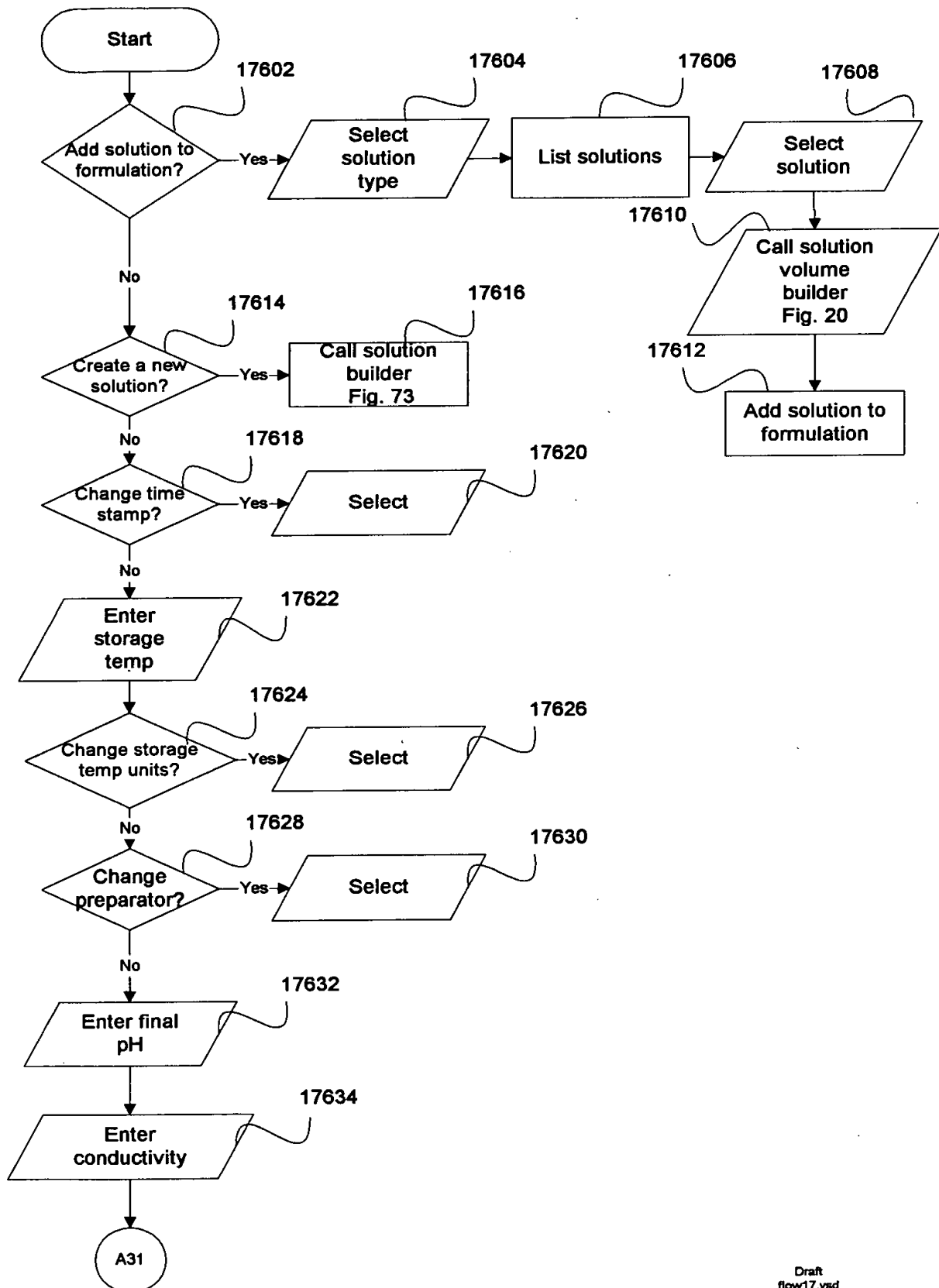


FIGURE 176

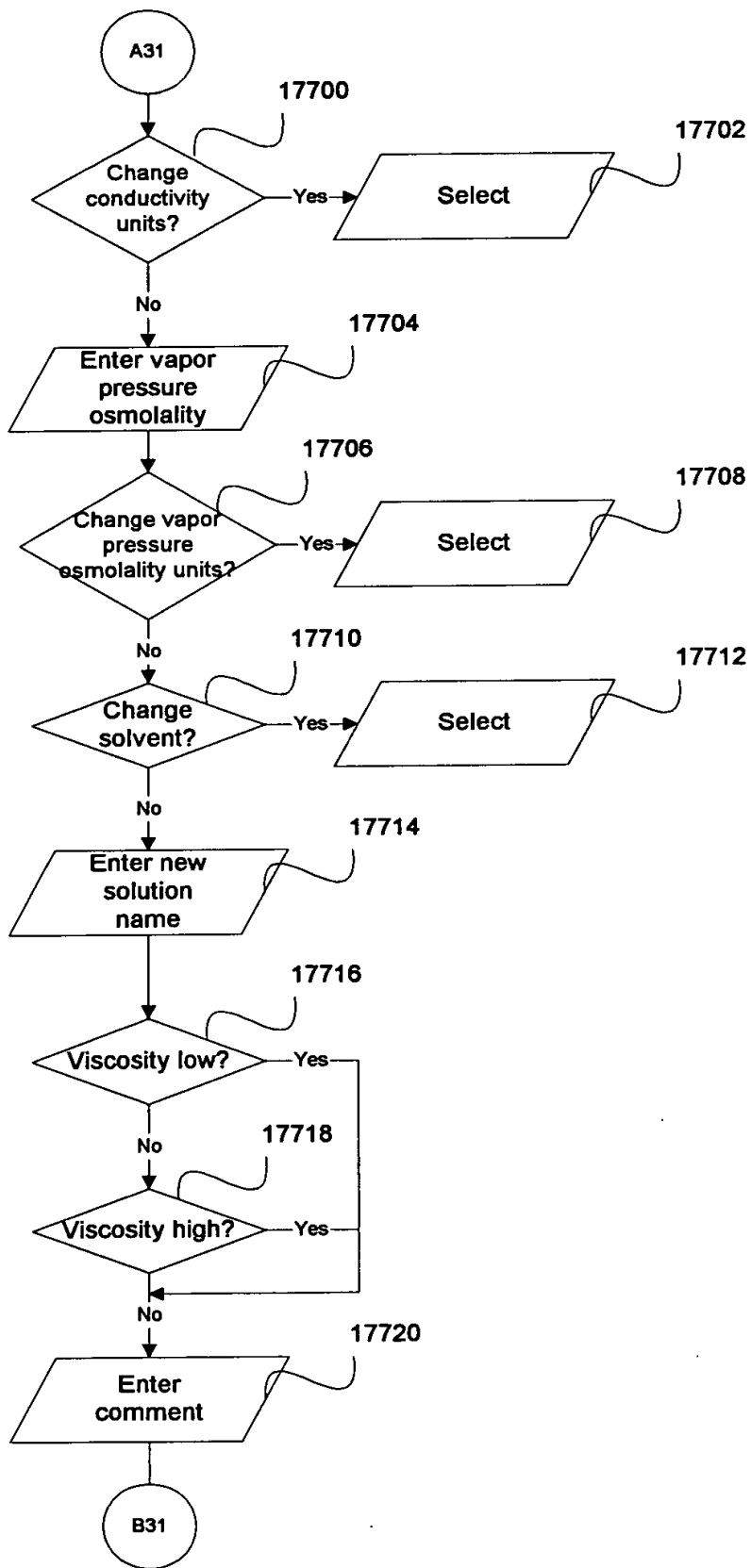
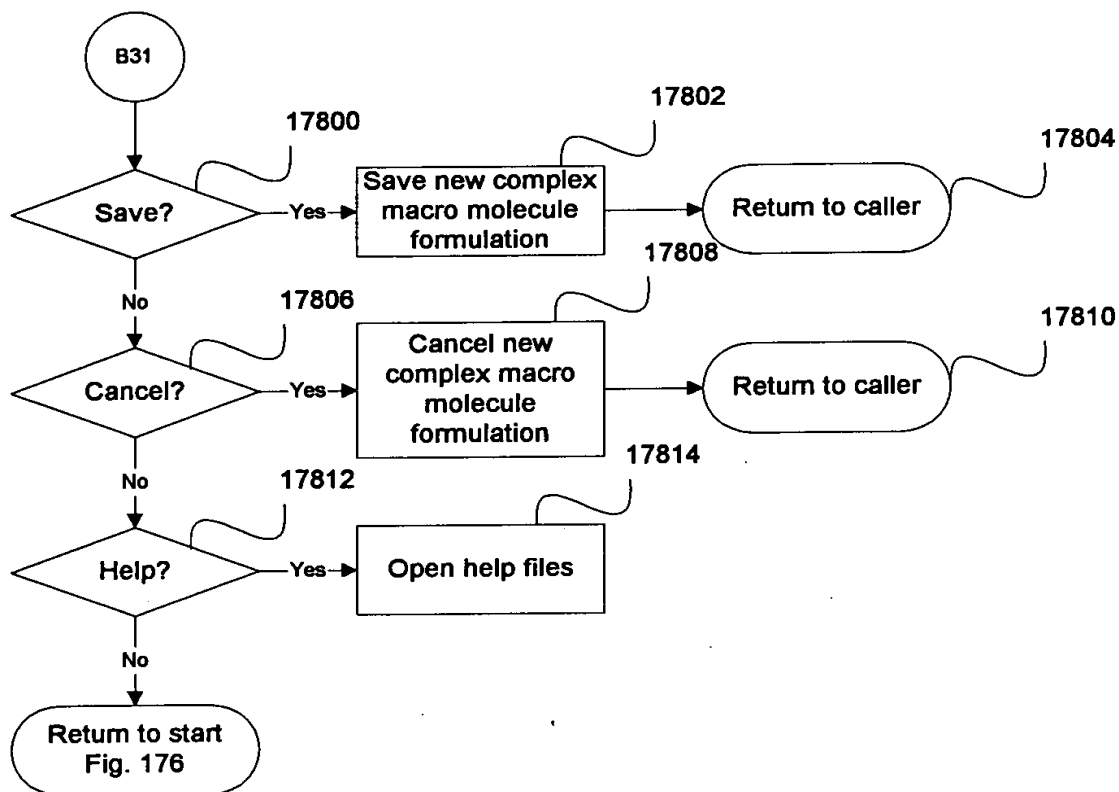
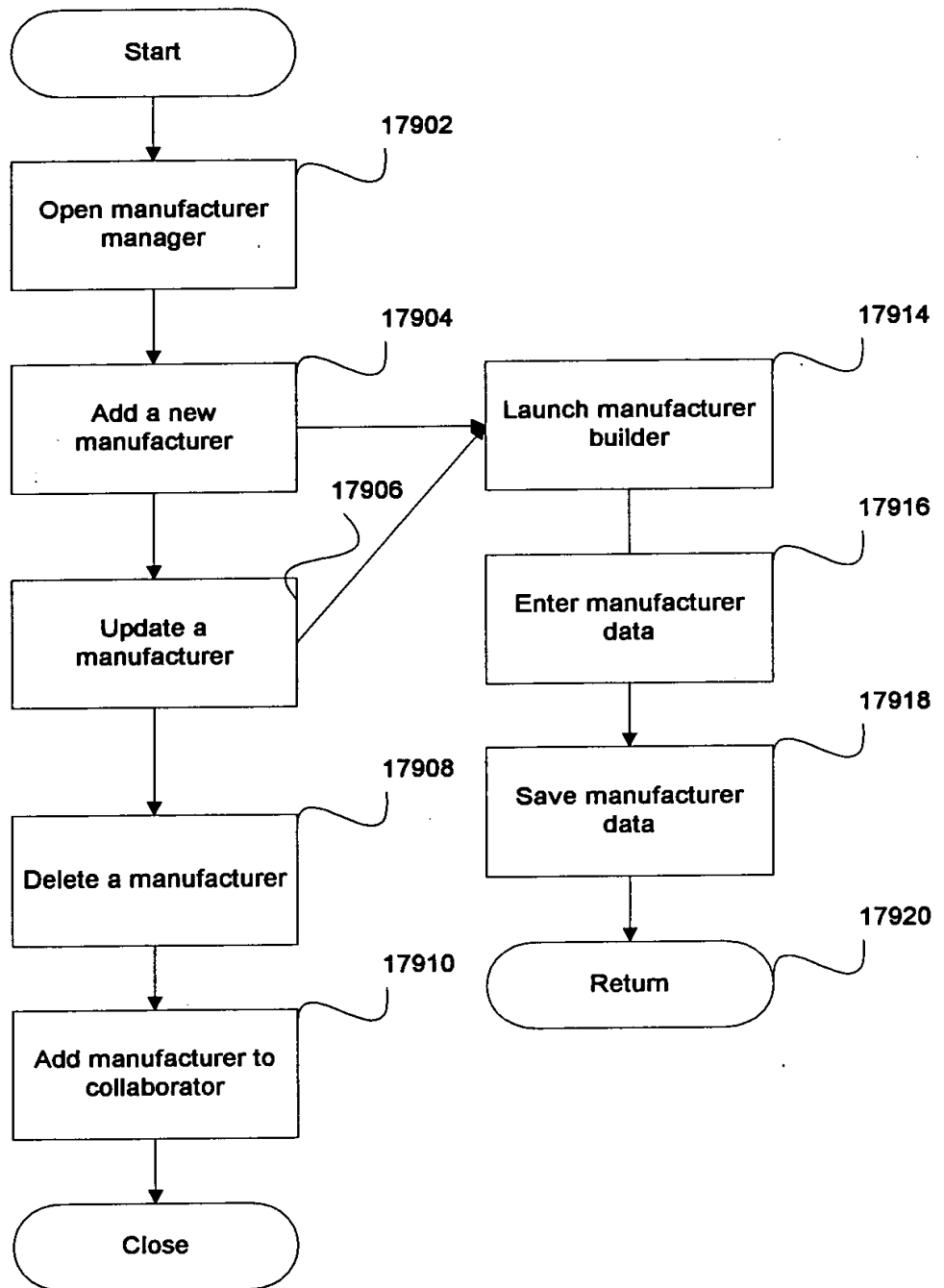


FIGURE 177

**FIGURE 178**



**FIGURE 179**






















18000

18001

002080" 58TTE80

### Manufacturer Manager

Name	Phone	Street	City
 Mother Earth	(800) 123-4567	Atmosphere and...	Milky Way
 Emerald BioStructures, Inc.	(888) 780-8535	7865 NE Day R...	Bainbridge Islar
 Sigma Chemical Co.	(800) 325-3010	P.O. Box 14508	St. Louis
 Fluka Chemical Corp.	(800) 358-5287	1001 W St. Paul...	Milwaukee
 Aldrich Chemical Co.	(800) 558-9160	P.O. Box 2060	Milwaukee
 Fisher Scientific Co.	(800) 766-7000	585 Alpha Dr.	Pittsburgh
 VWR Scientific Products Co...	(800) 932-5000	1310 Goshen P...	West Chester
 J. T. Baker	(800) 582-2537	222 Red School...	Phillipsburg
 Promega Corp.	(800) 356-9526	2800 Woods Ho...	Madison
 Pierce Chemical Co.	(800) 874-3723	3747 N Meridian...	Rockford
 Mallinckrodt	(800) 354-2050	222 Red School...	Phillipsburg
 ICN Pharmaceuticals, Inc.	(800) 854-0530	3300 Hyland Ave.	Costa Mesa
 Bio-Rad Laboratories	(800) 424-6723	2000 Alfred Nob...	Hercules
 Amersham Pharmacia Biote...	(800) 526-3593	800 Centennial ...	Piscataway
 Invitrogen Corp.	(800) 955-6288	1600 Faraday A...	Carlsbad
 Calbiochem-Novabiochem C...	(800) 854-3417	P.O. Box 12087	La Jolla
 Hampton Research Corp.	(800) 452-3899	27632 El Lazo Rd.	Laguna Niguel

18002

18004

18006

18008

18010

18012

New...

Update...

Delete

Add to Collab

Help...

Close

FIG. 180

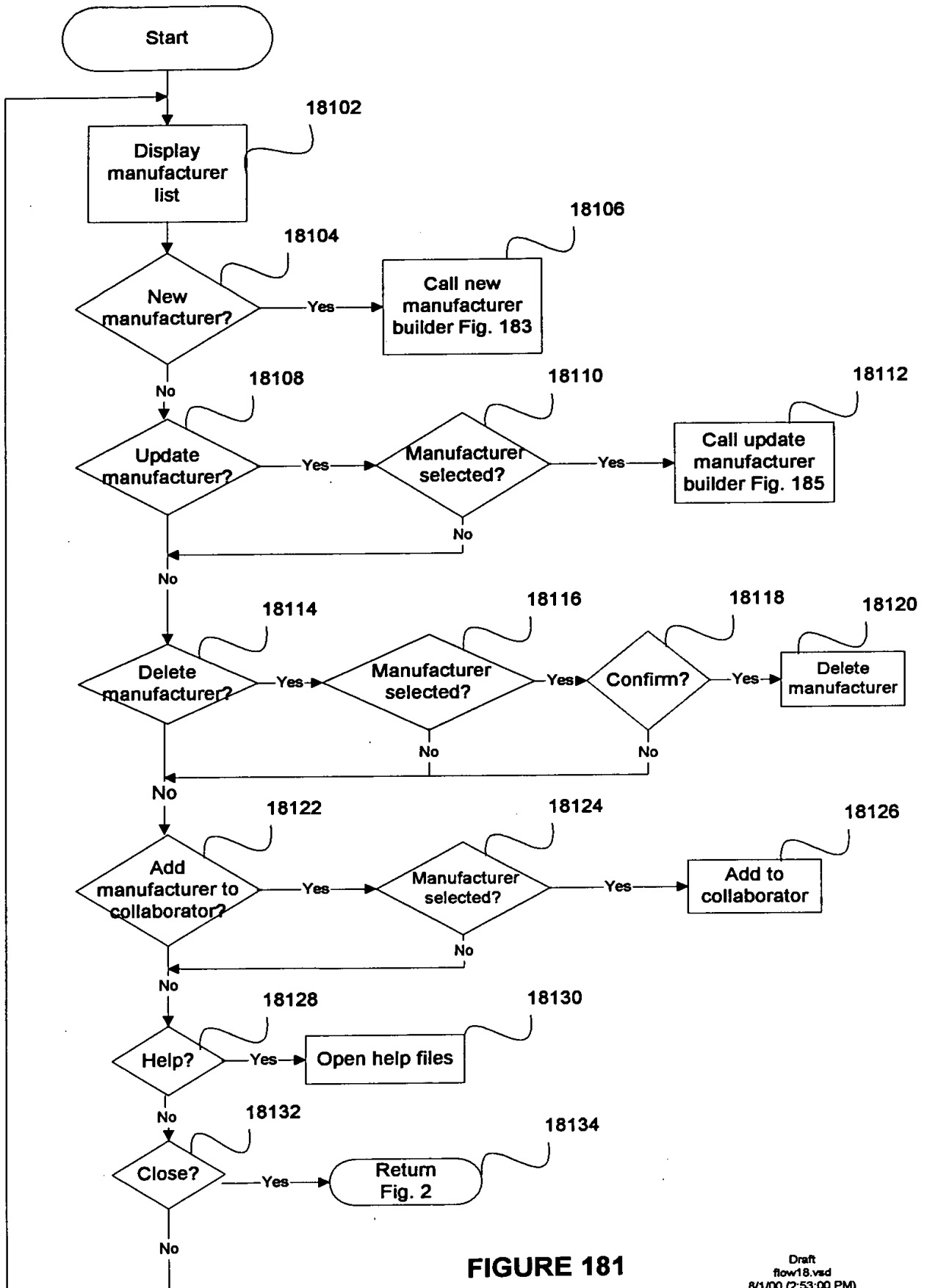


FIGURE 181

Update Emerald BioStructures, Inc. [X]

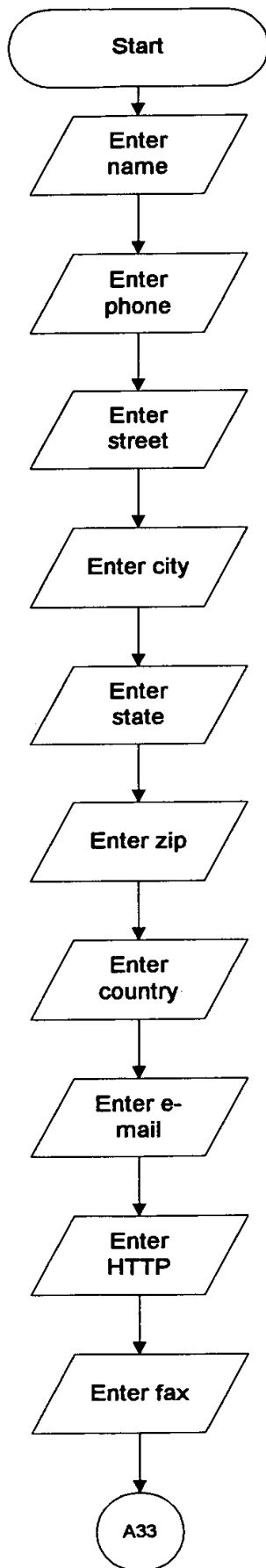
Name:	Emerald BioStructures, Inc.	18200
Phone:	(888) 780-8535	18202
Street:	7865 NE Day Rd. W	18204
City:	Bainbridge Island	18206
State:	WA	18208
Zip:	98110	18210
Country:	USA	18212
Email:	info@emeraldbiostructures.com	18214
HTTP:	http://www.emeraldbiostructures.com	18216
Fax:	(206) 780-8549	18218
Dept:		18220

OK Cancel

18224 18226

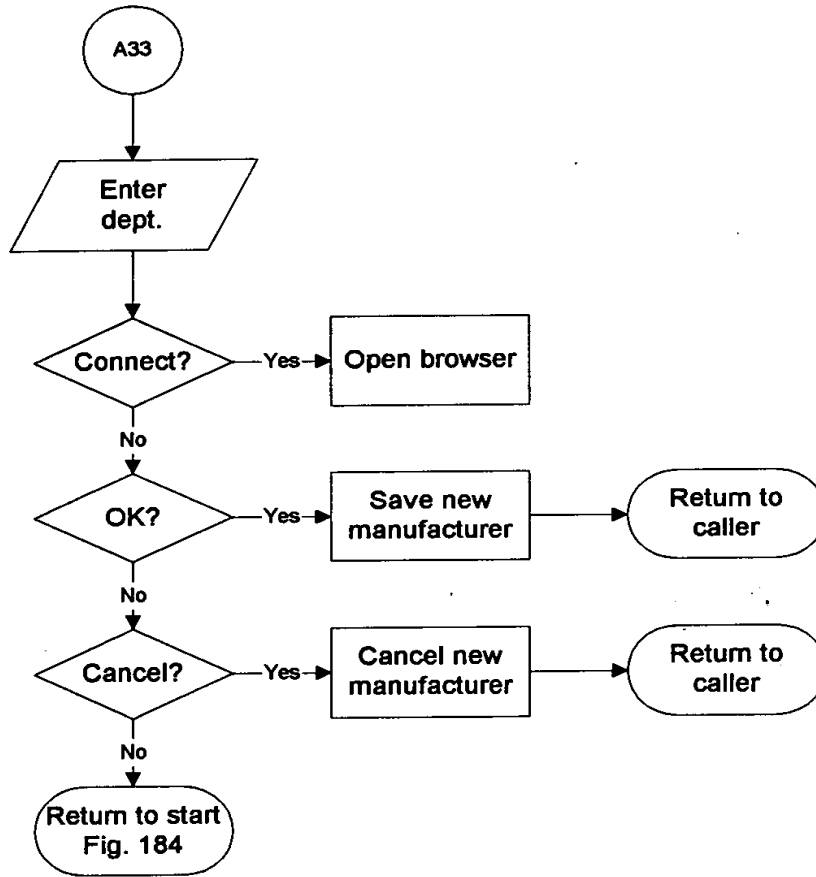
Fig. 182

002080 "EST" 960



**FIGURE 183**

002020 "ESTEC360



**FIGURE 184**

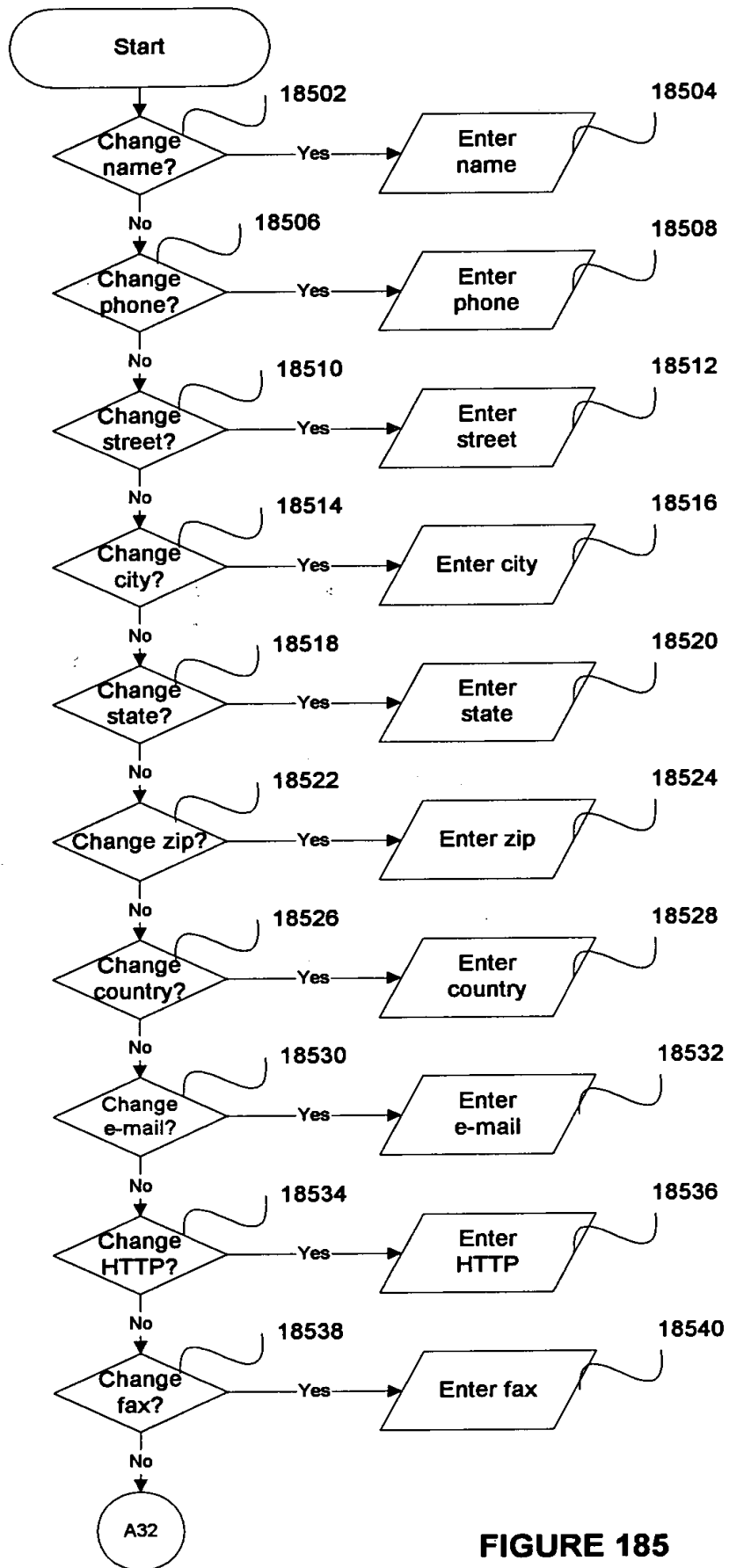


FIGURE 185

002030" 53T1E960

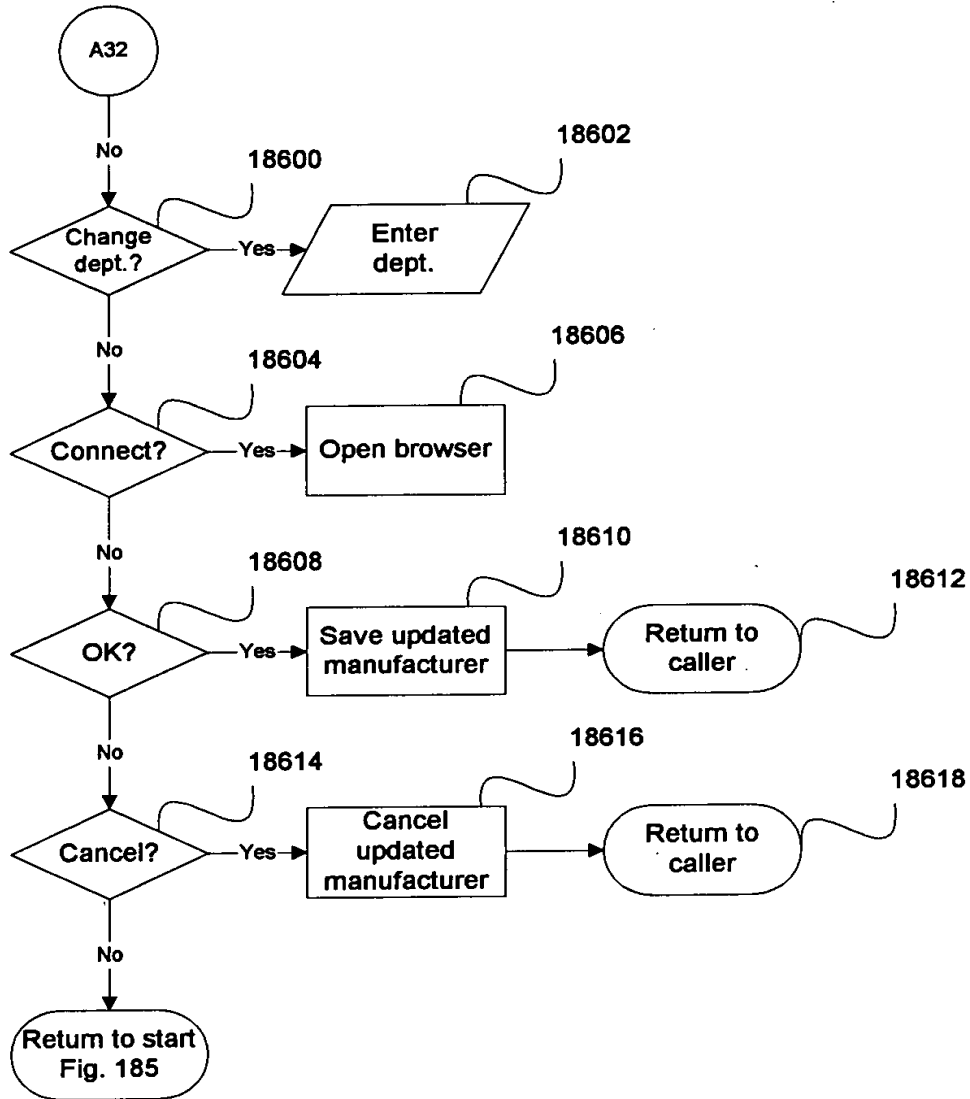
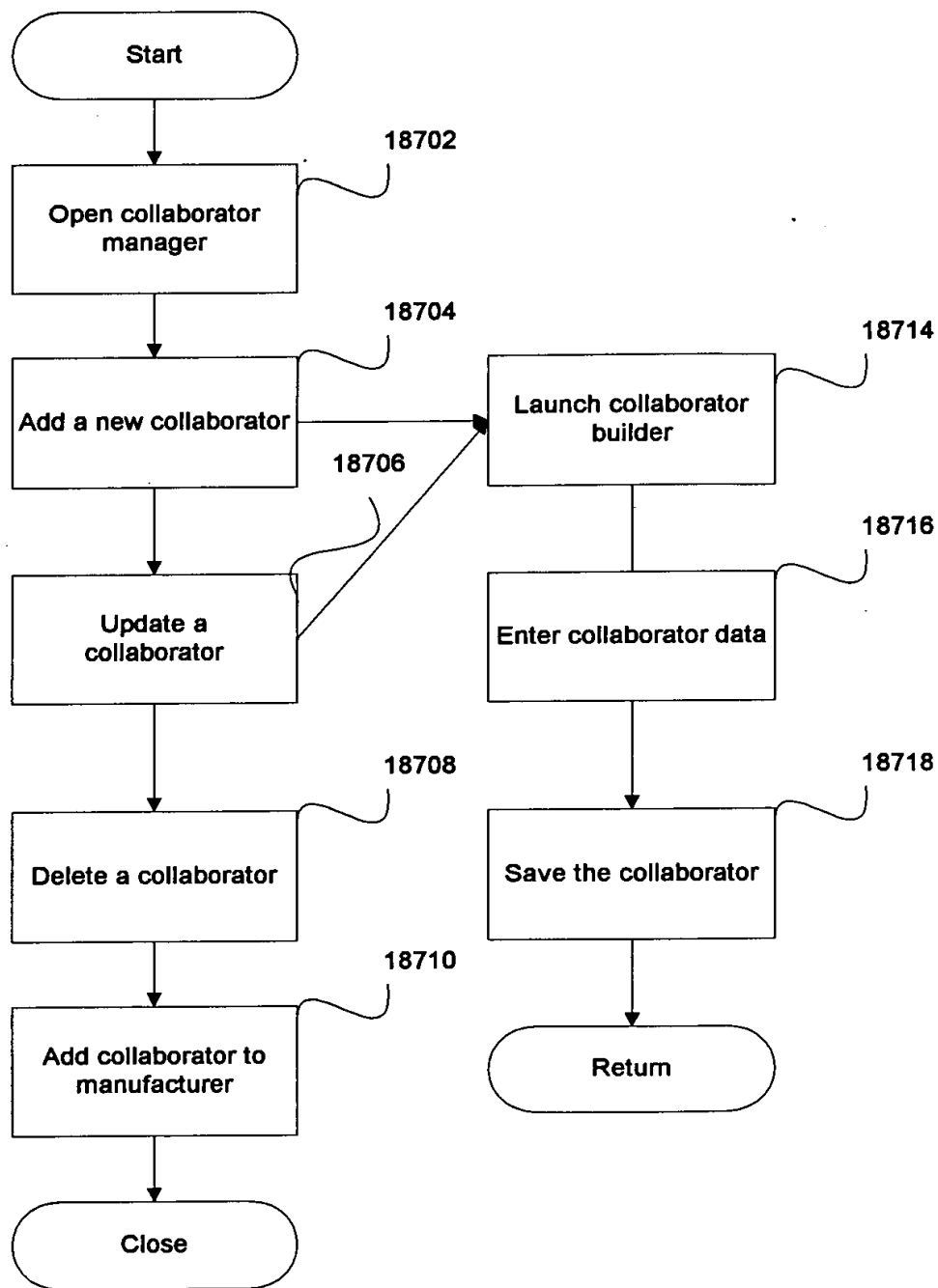


FIGURE 186



**FIGURE 187**



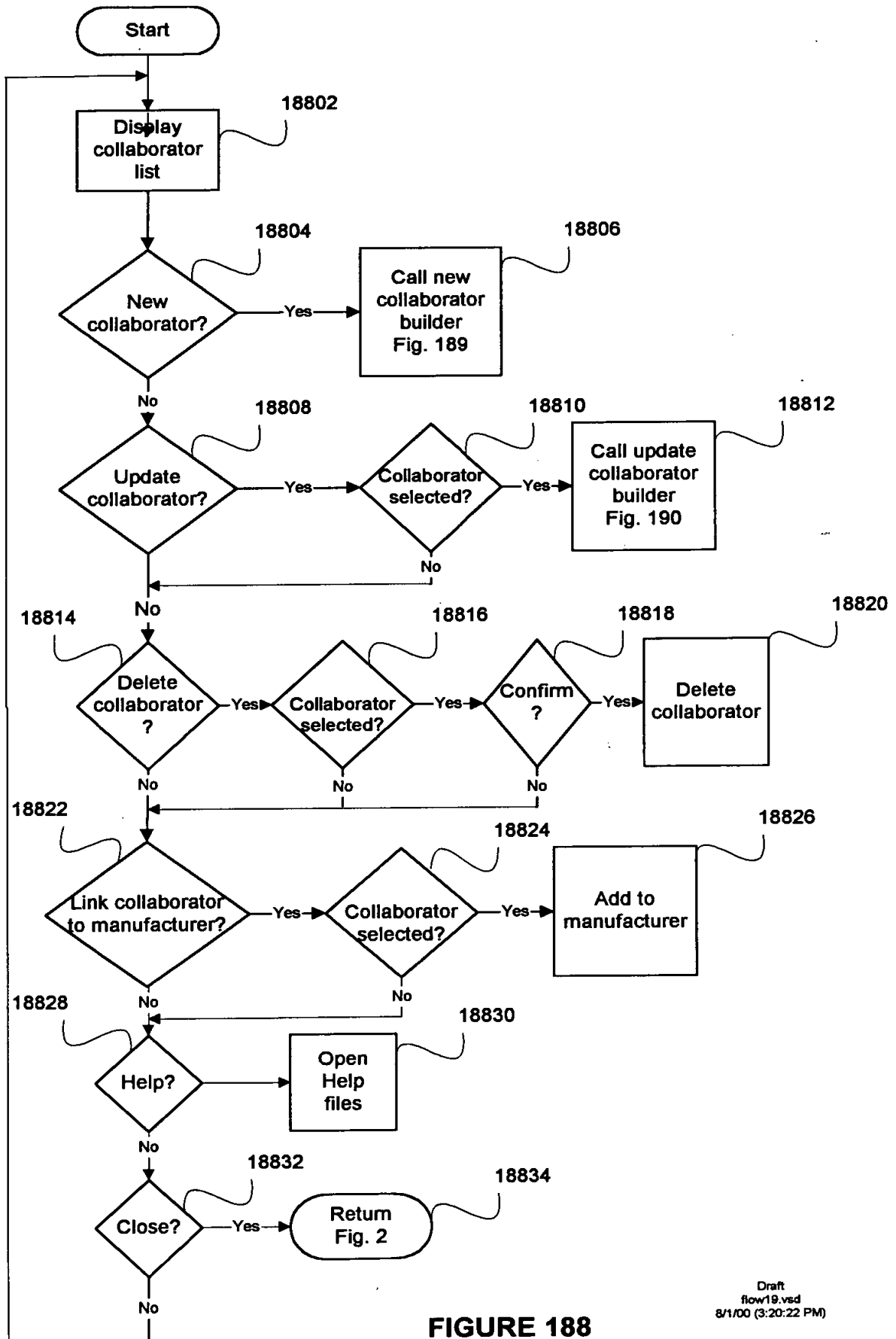


FIGURE 188

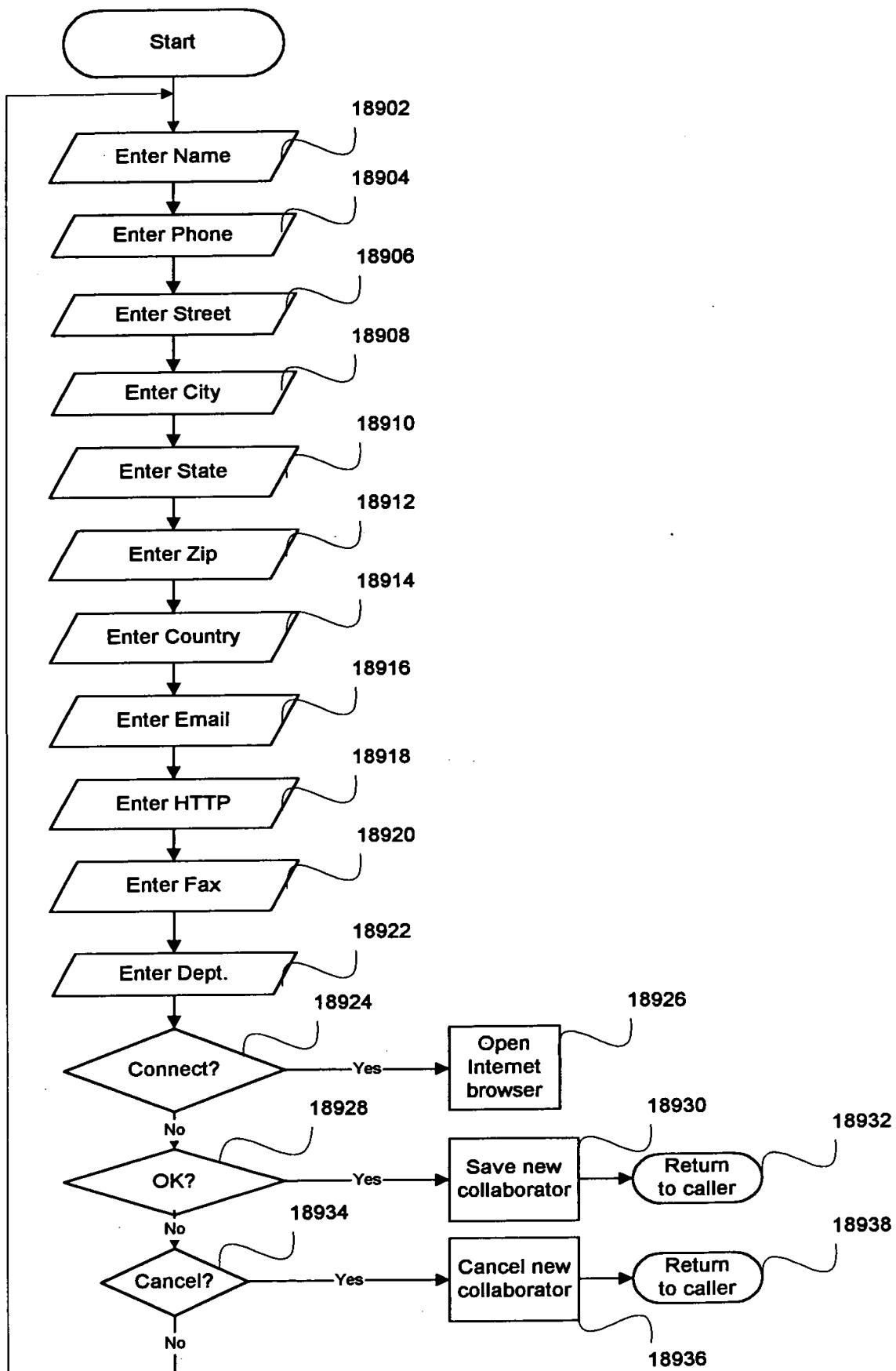


FIGURE 189

002090" ESTE 960

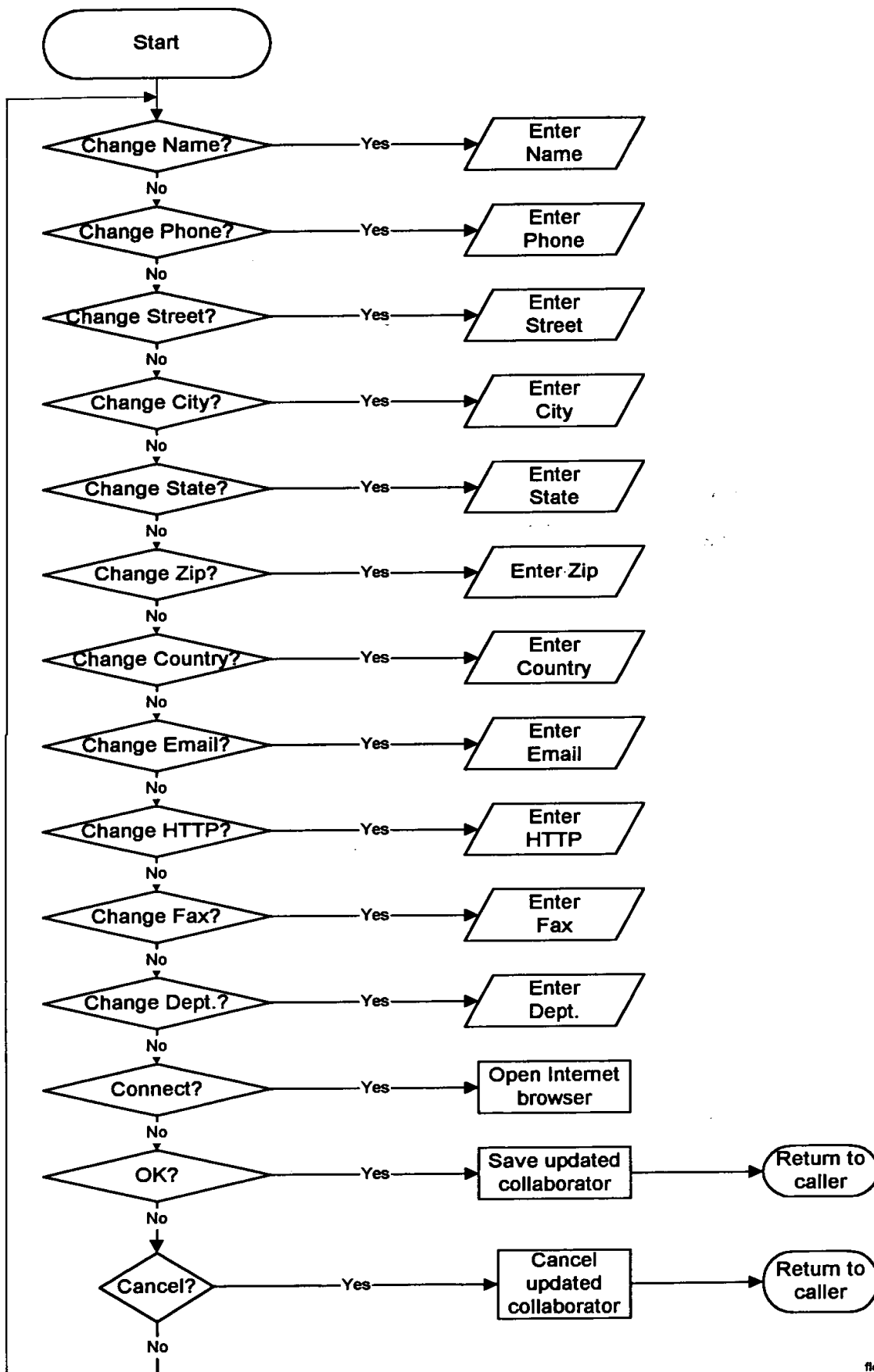


FIGURE 190

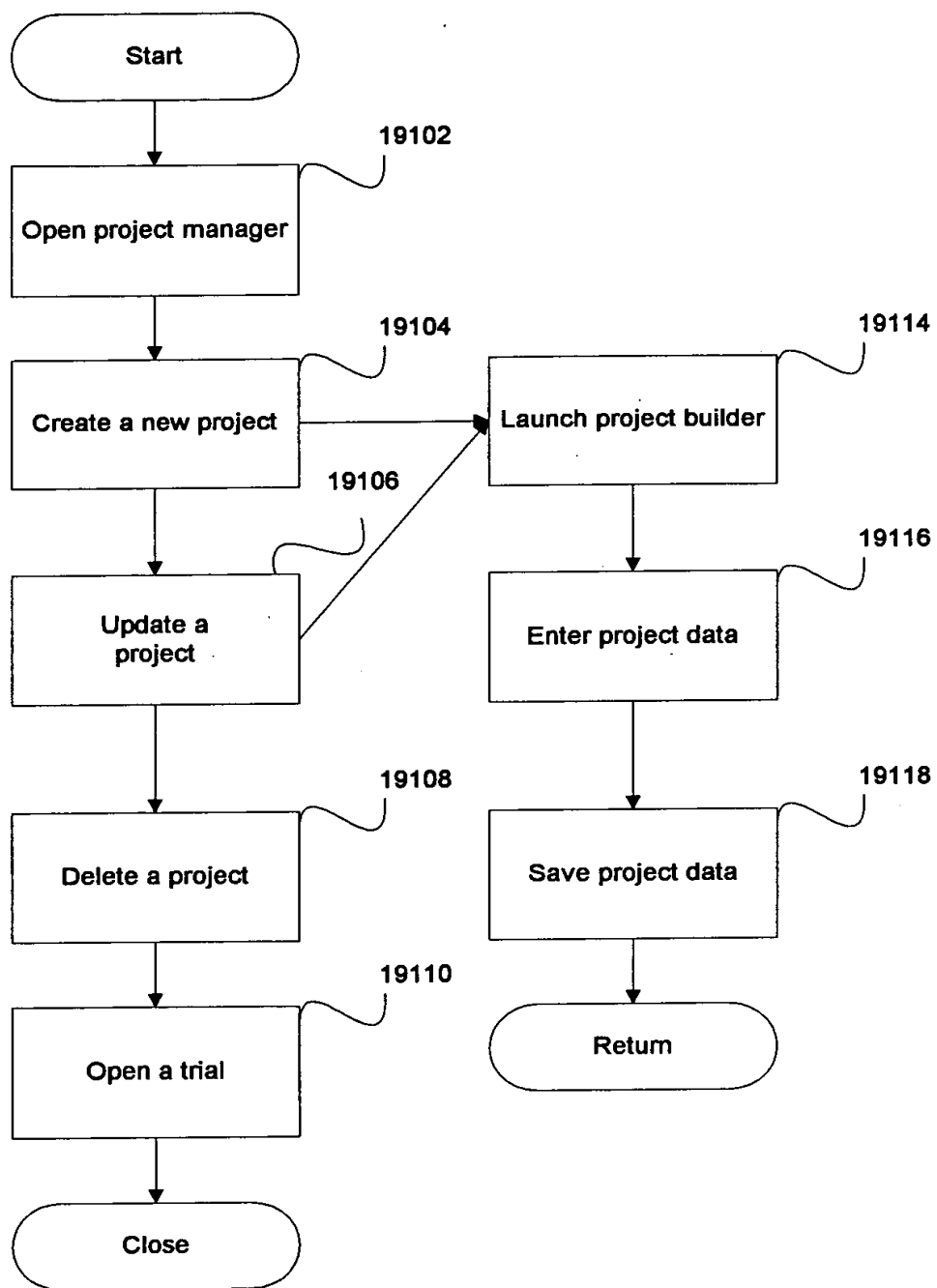


FIGURE 191

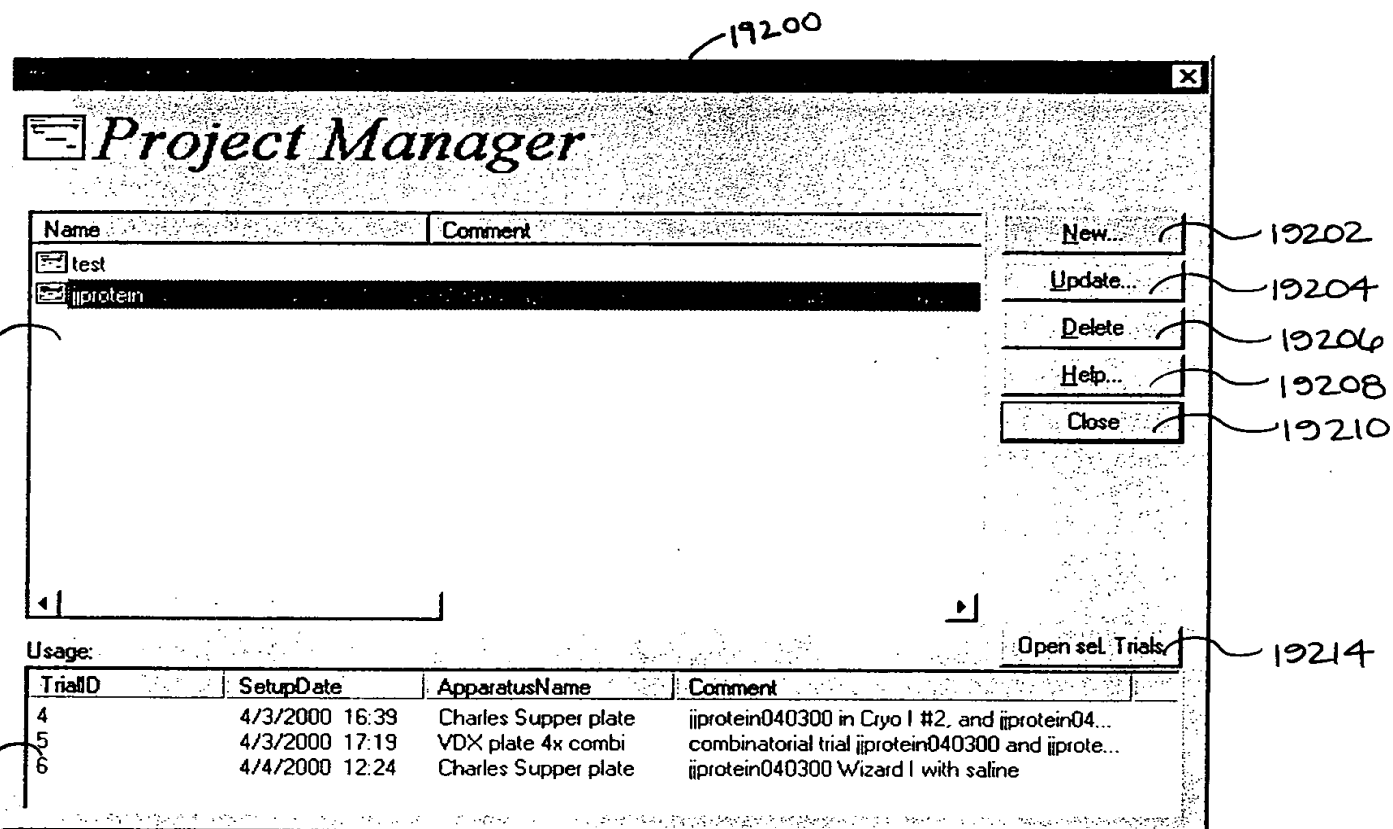


Fig. 192

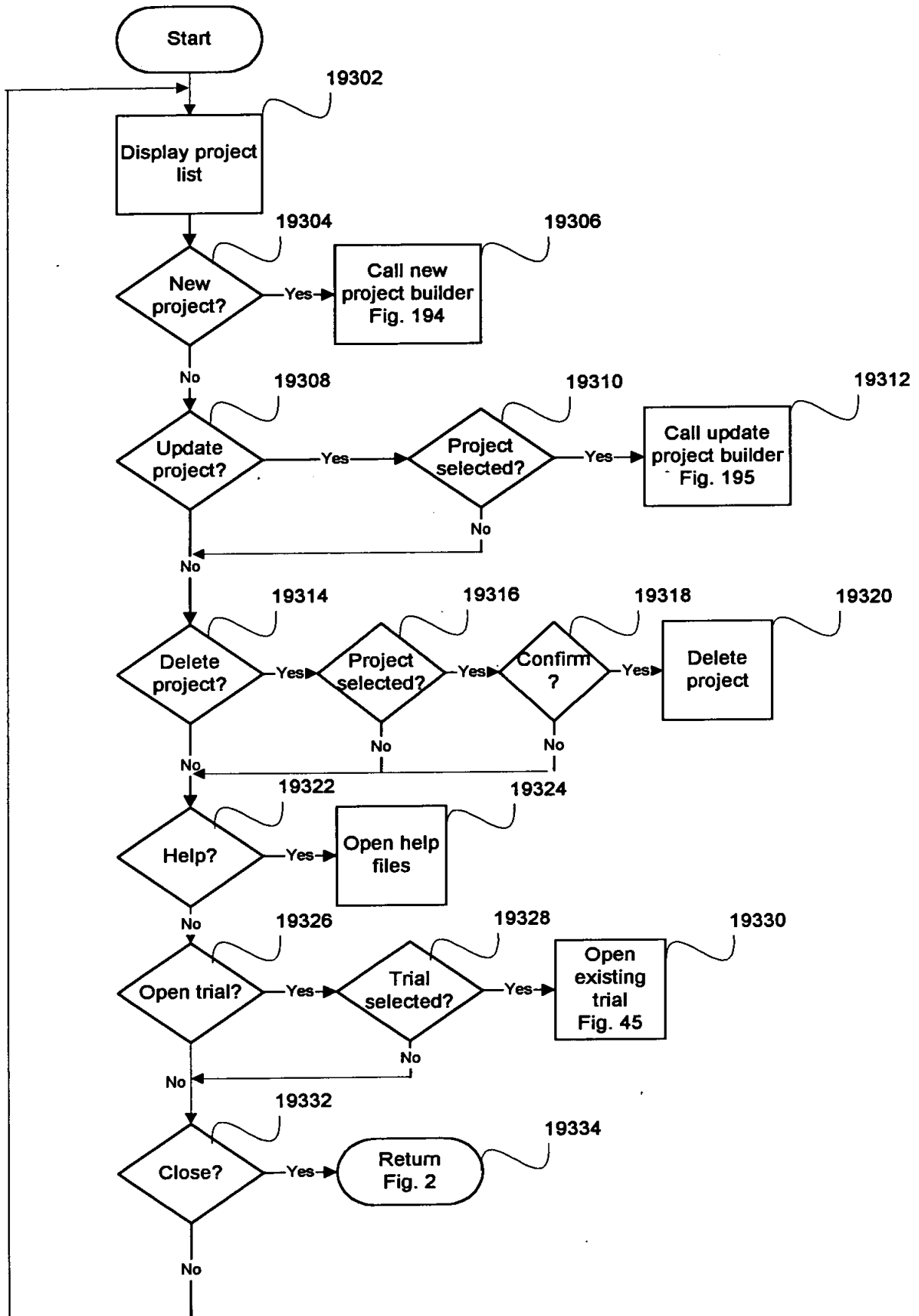


FIGURE 193

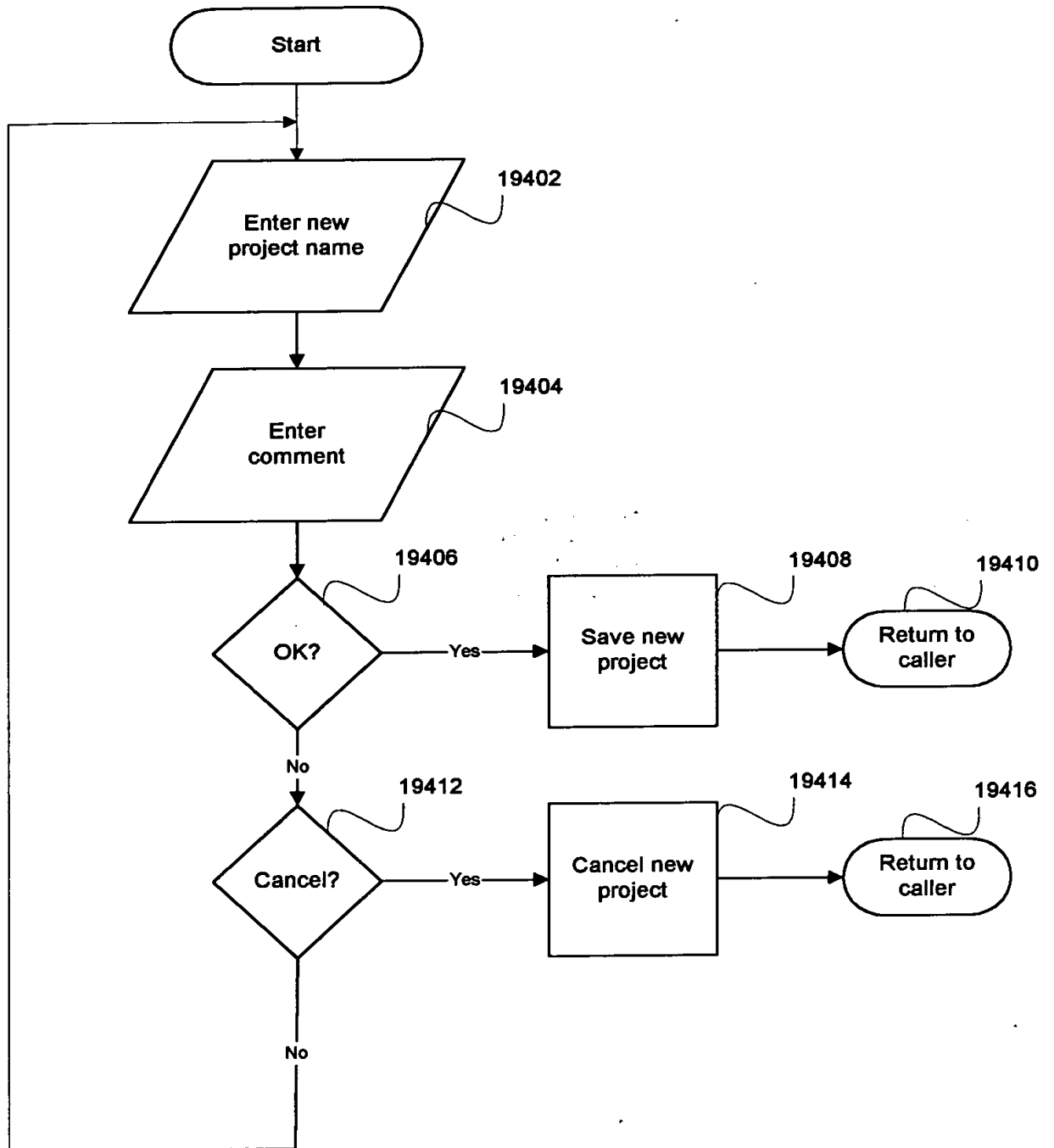


FIGURE 194

002090" SST E960

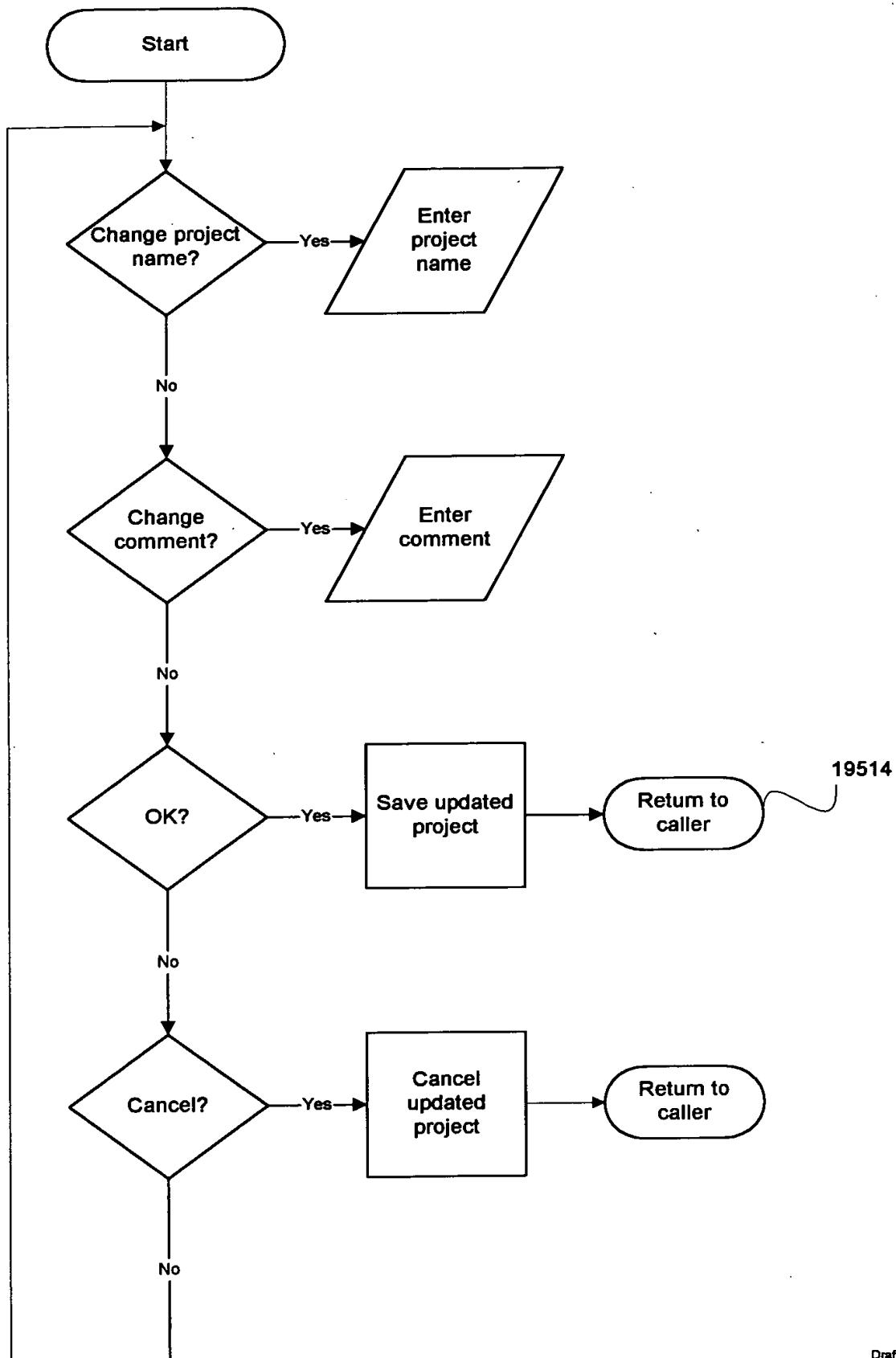
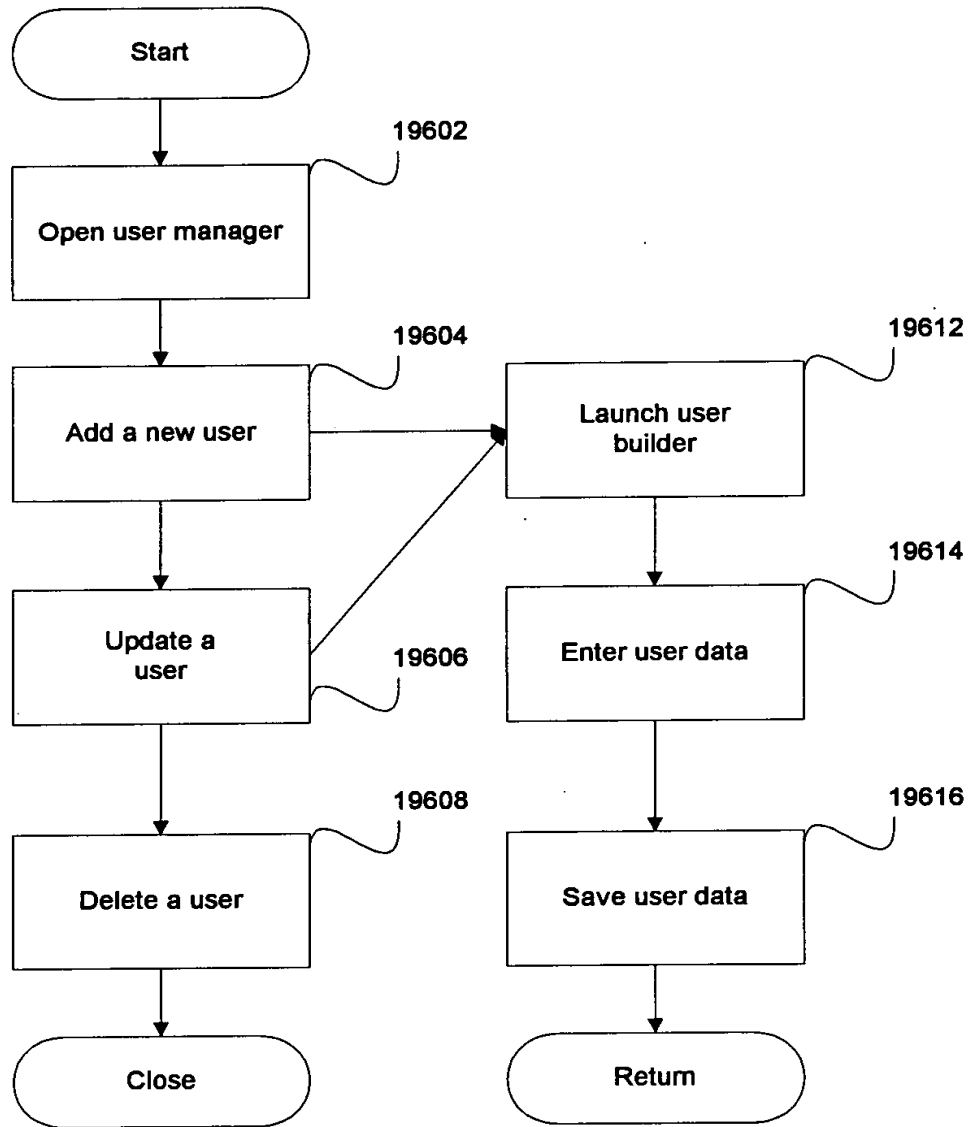


FIGURE 195





**FIGURE 196**

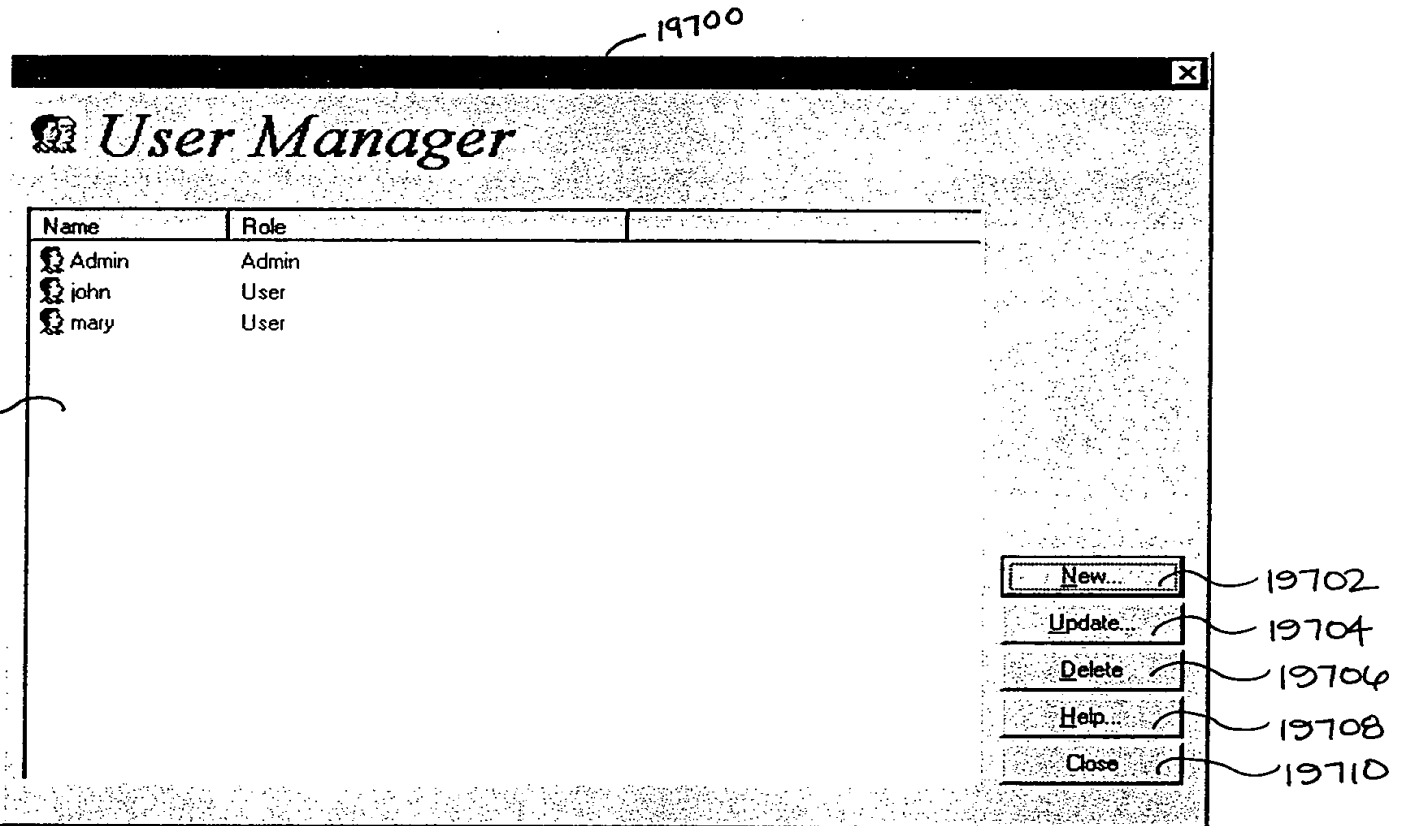


FIG. 197

002080" SSTF 960

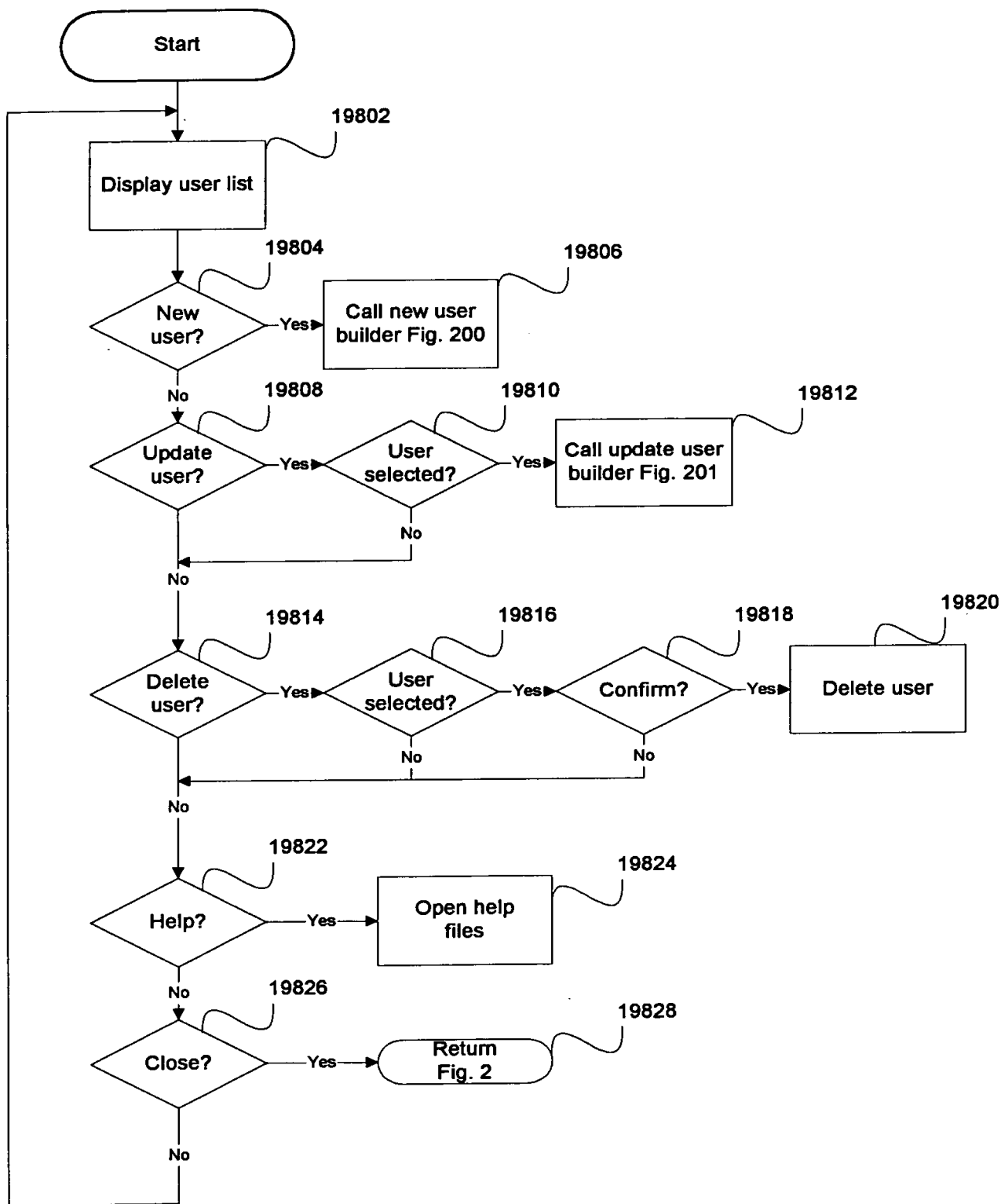


FIGURE 198

002080" 587E960

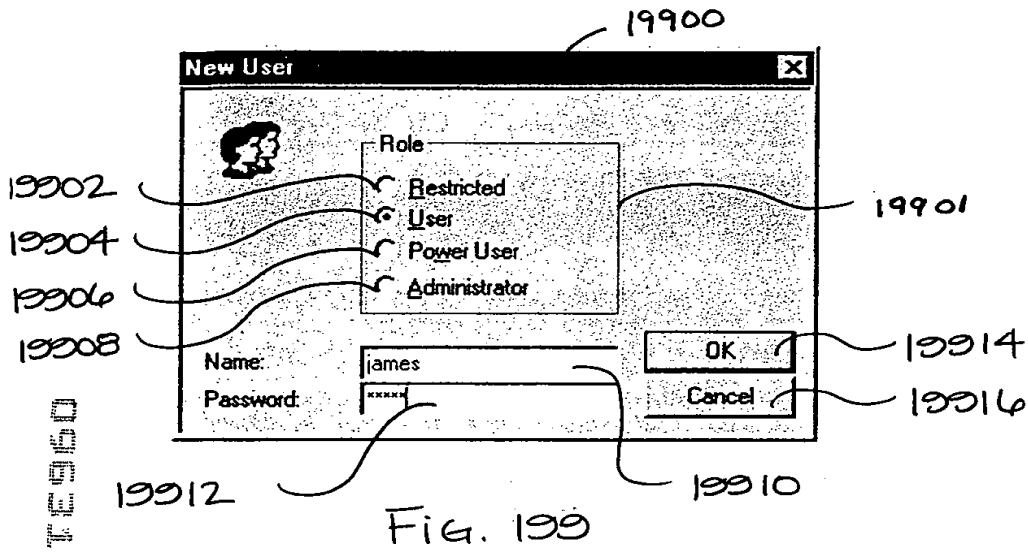


Fig. 199

002080" 55TTE960

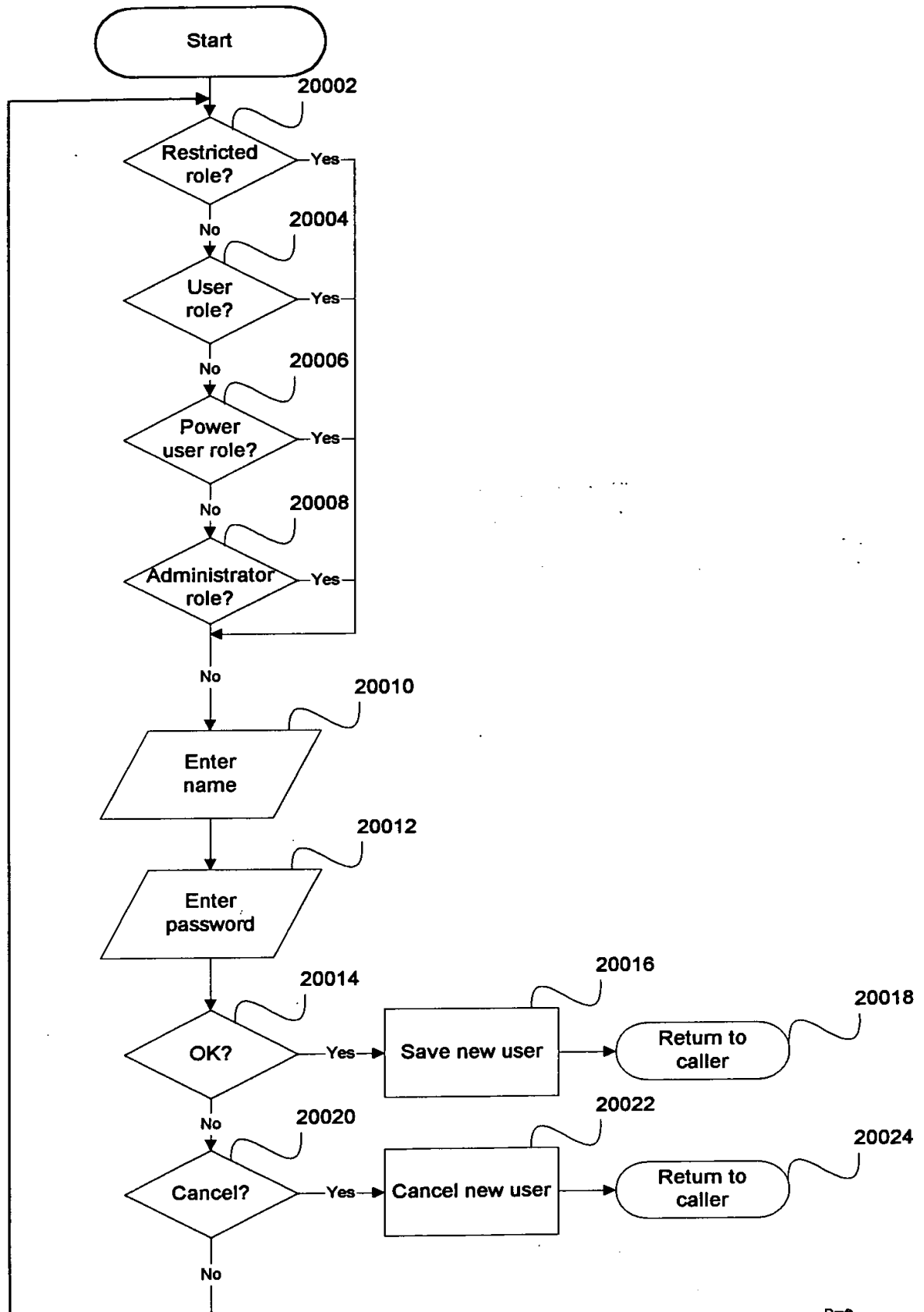


FIGURE 200

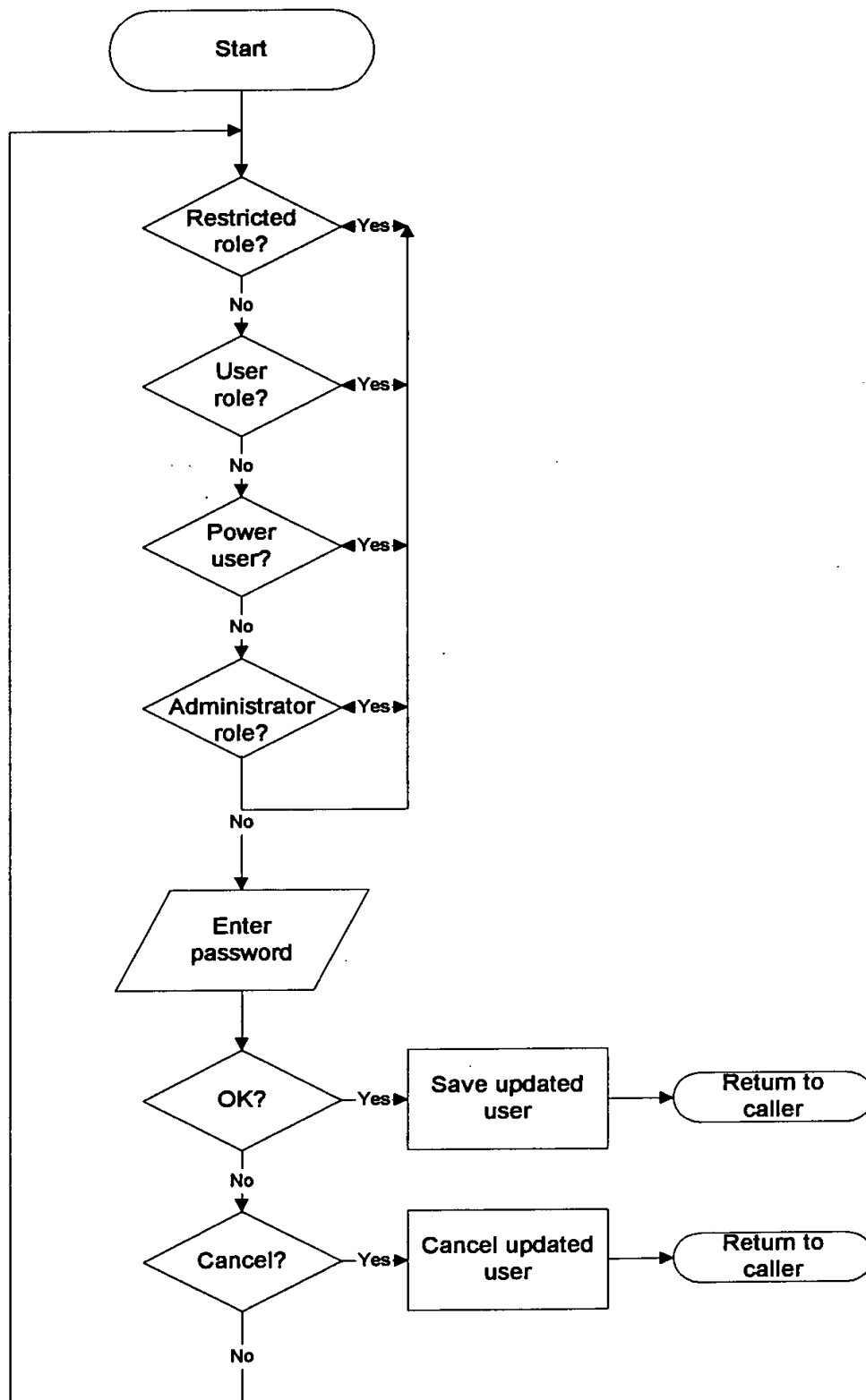
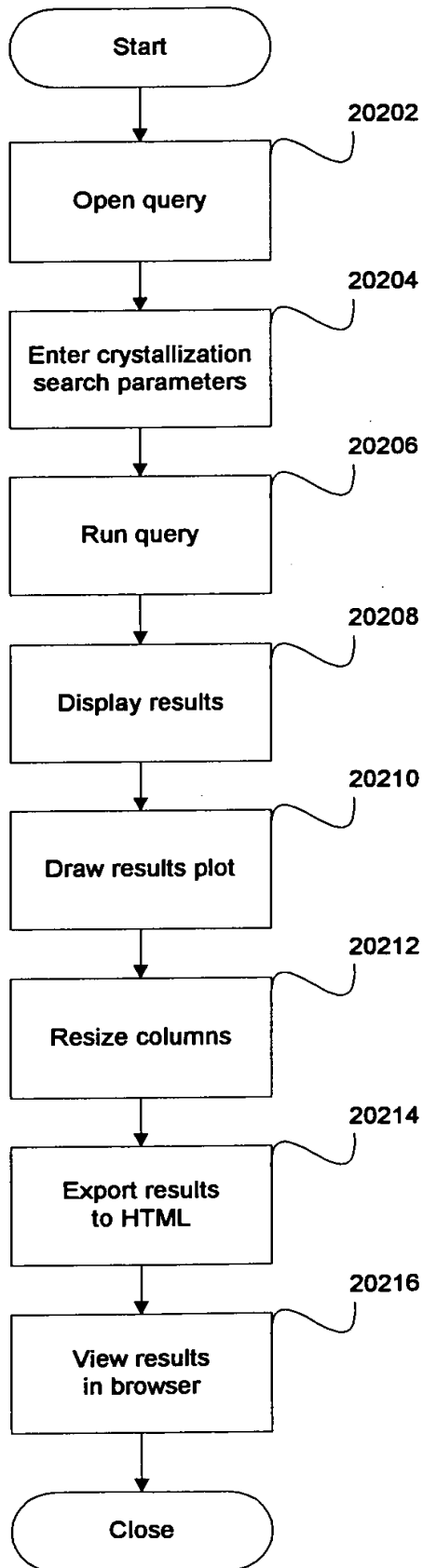


FIGURE 201



**FIGURE 202**



0963135-080200

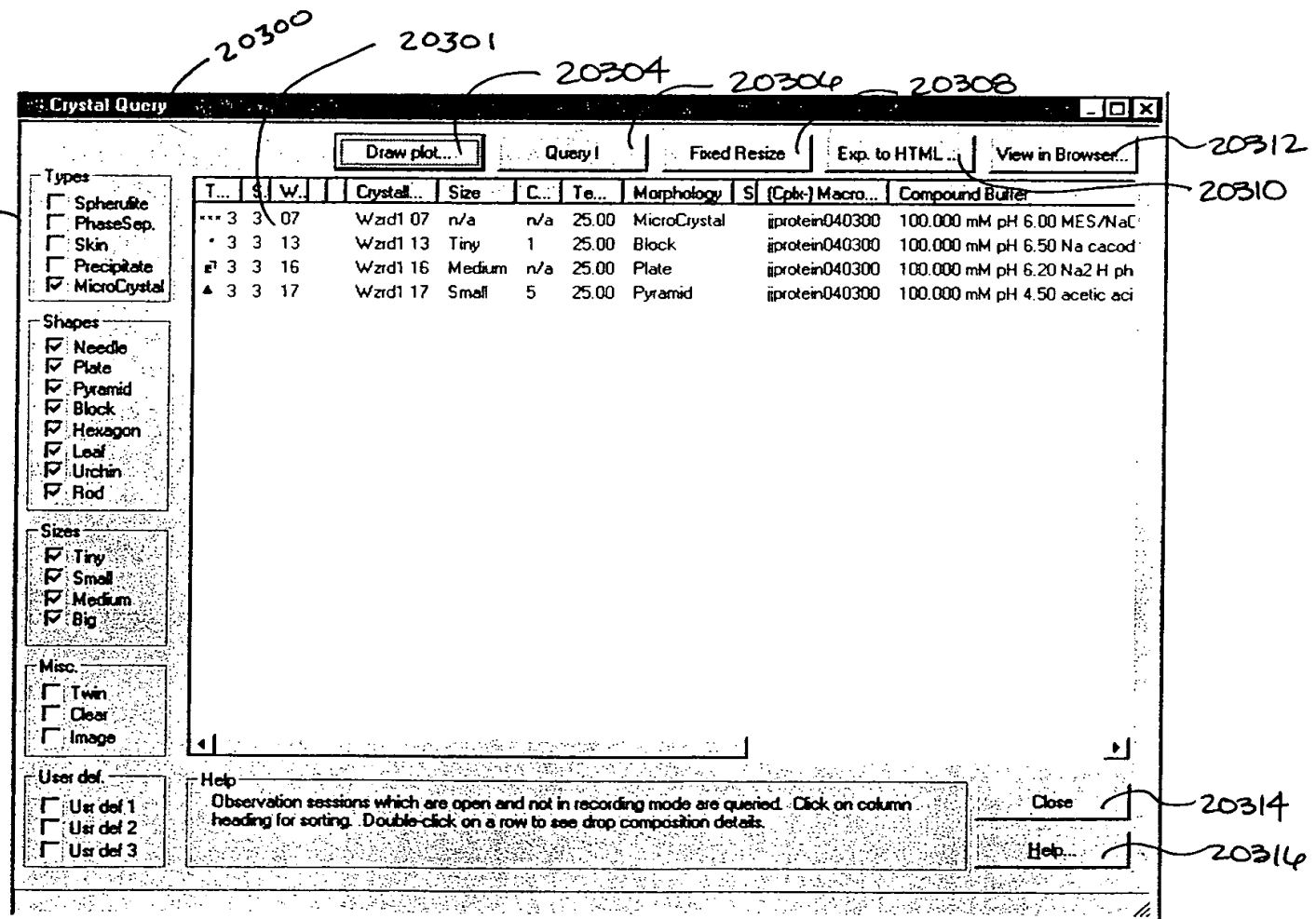


Fig. 203



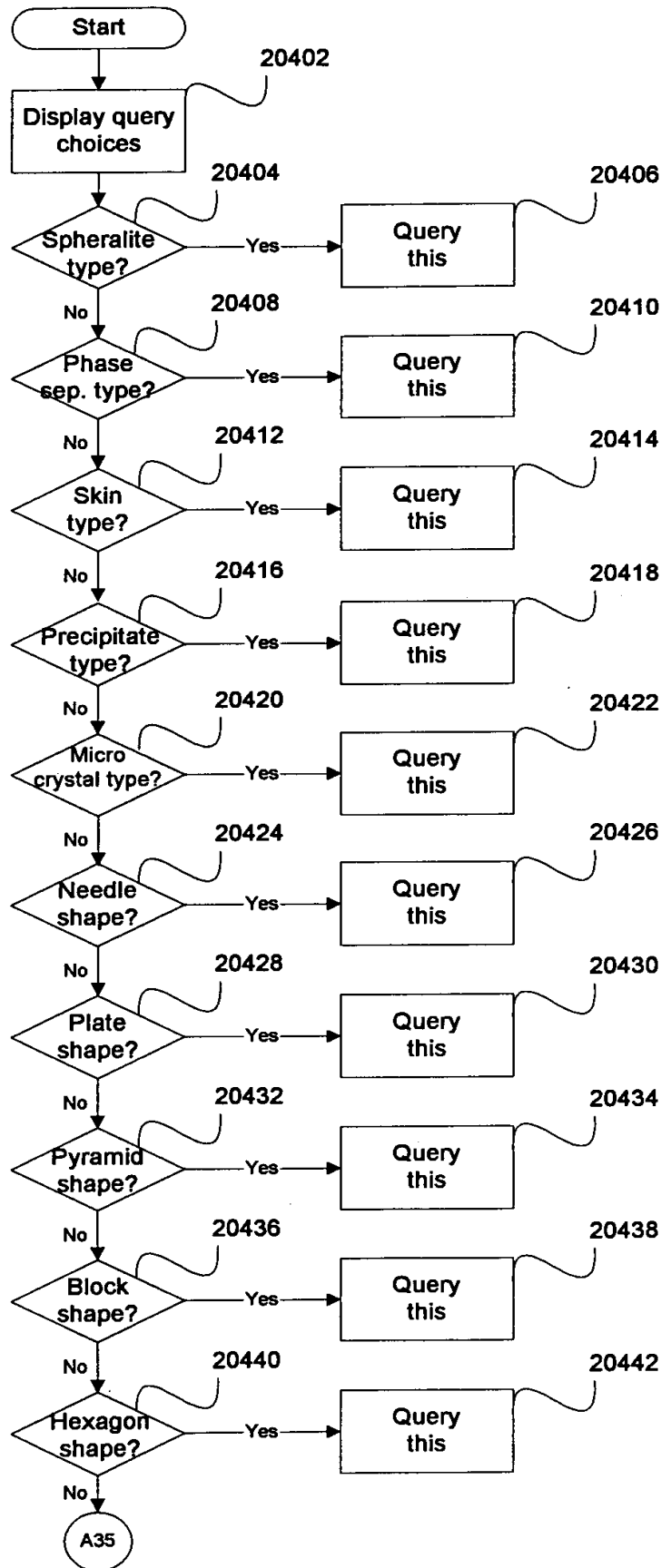


FIGURE 204

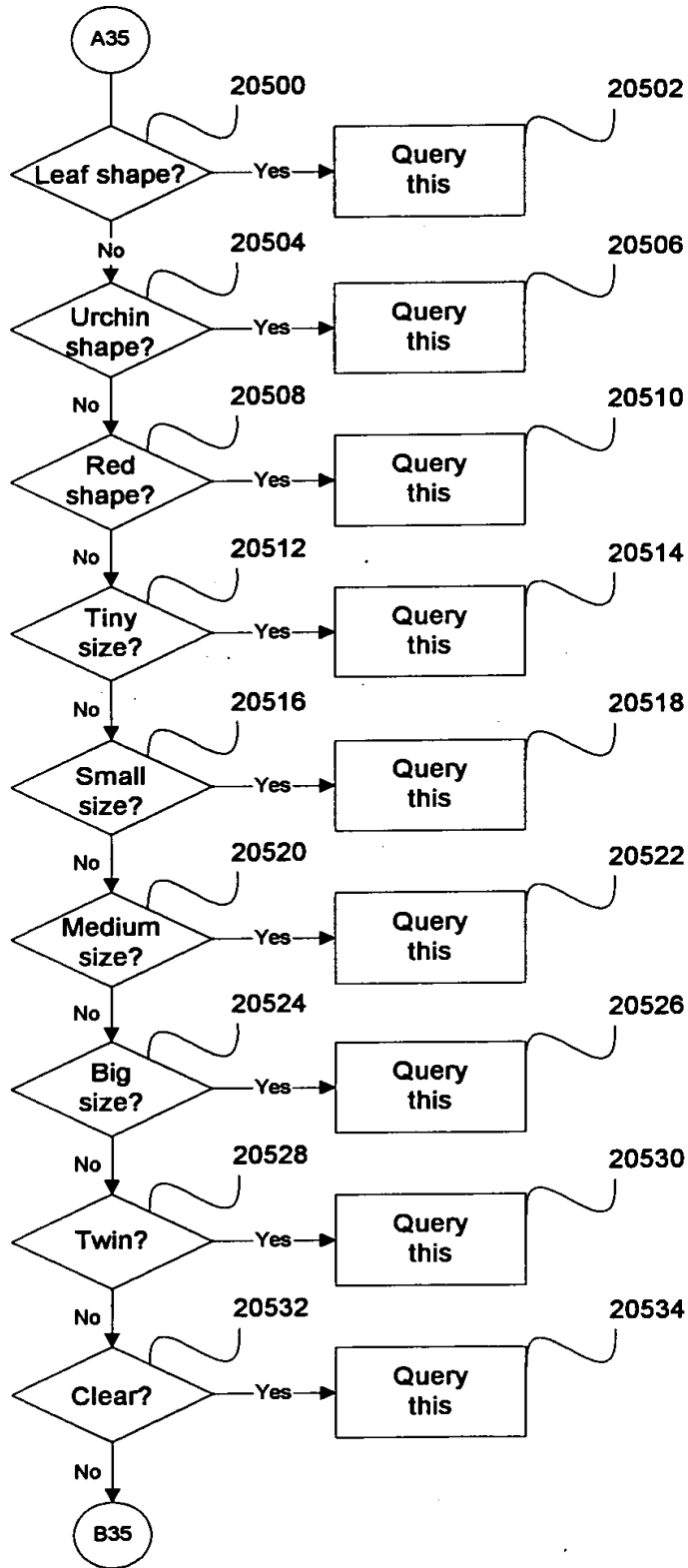


FIGURE 205

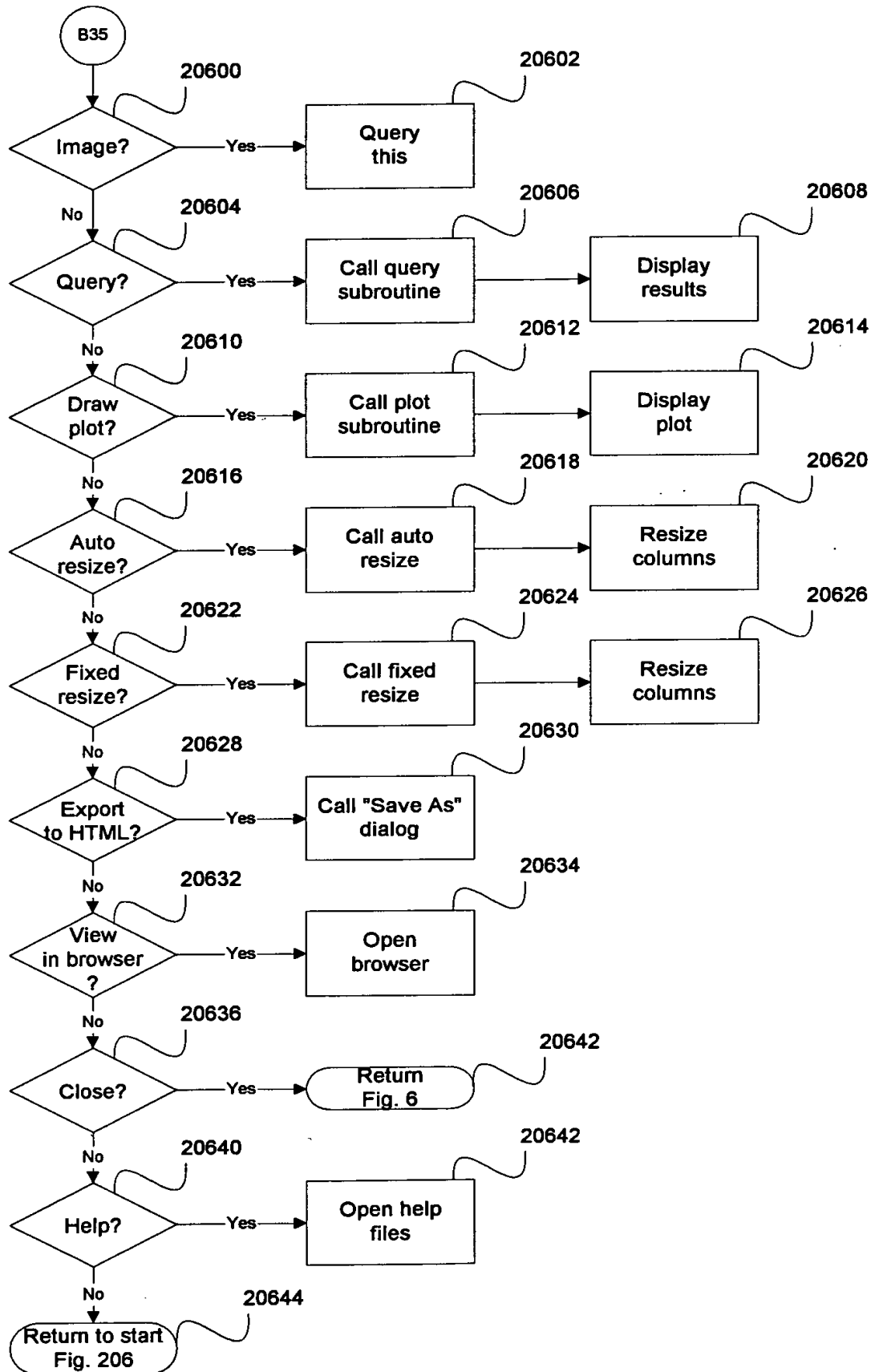
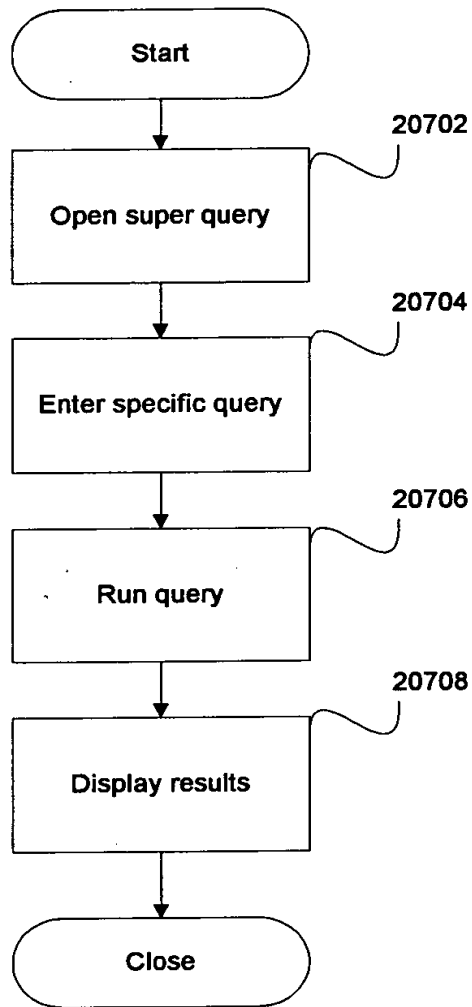


FIGURE 206



**FIGURE 207**



20800

20802

20801

Crystal Monitor Super Query

Query #1: Show me all Trials where Crystals were obtained in the presence of the following chemical:

Catalog: 81268 CAS: 25322-68-3 Query 20806

TrialID	SetupDate	MatrixName	ProjectName	ApparatusName
3	4/3/2000 16:10	Wzrd1	test	Charles Supper ...

20804

Notes

The super query is only a technology preview. Only one query is implemented. Many other queries will follow, once enough feedback has been collected from customers. Please send any query request to support@emeraldstructures.com.

OK 20808

Cancel 20810

Help... 20812

Fig. 208

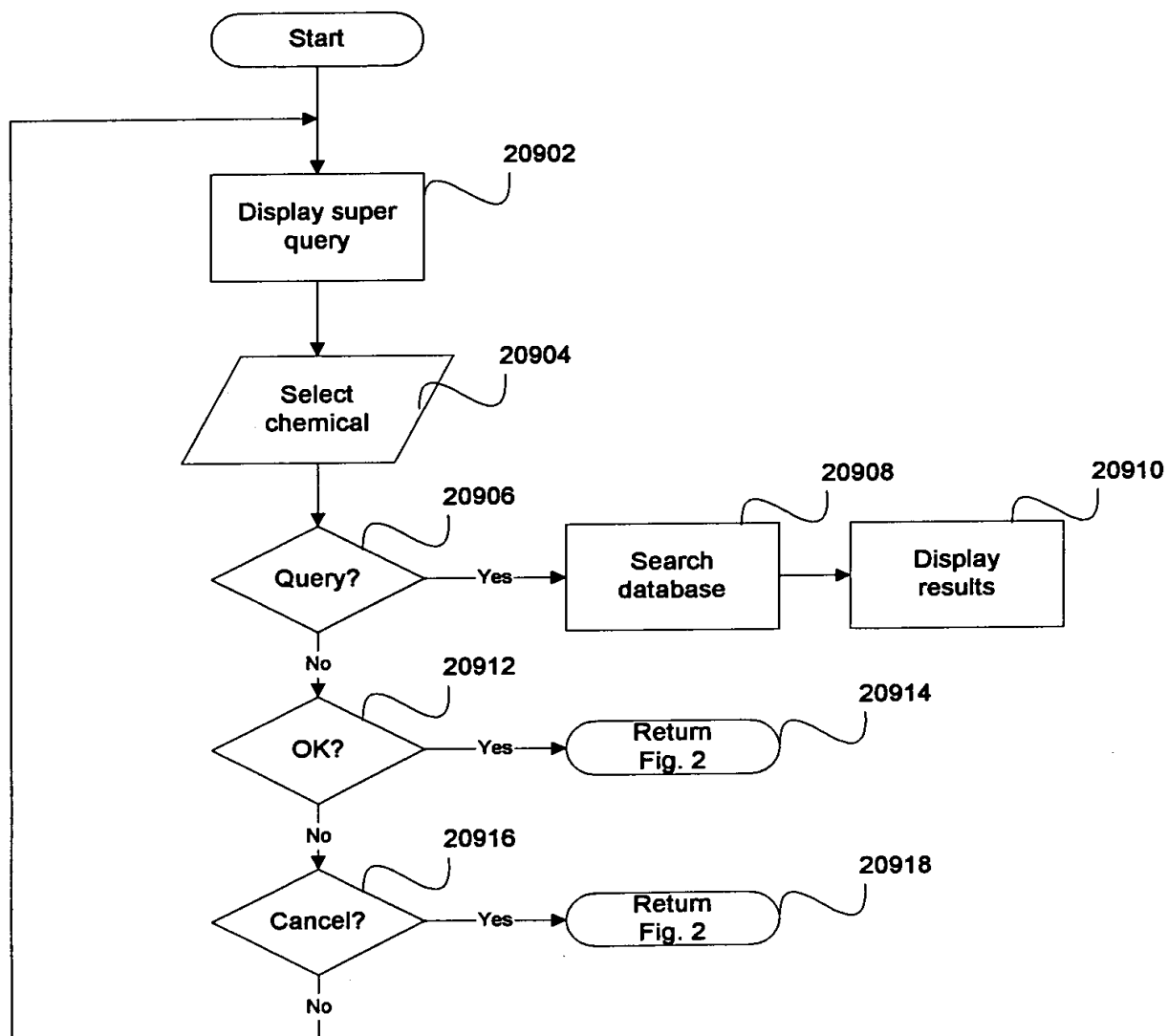


FIGURE 209

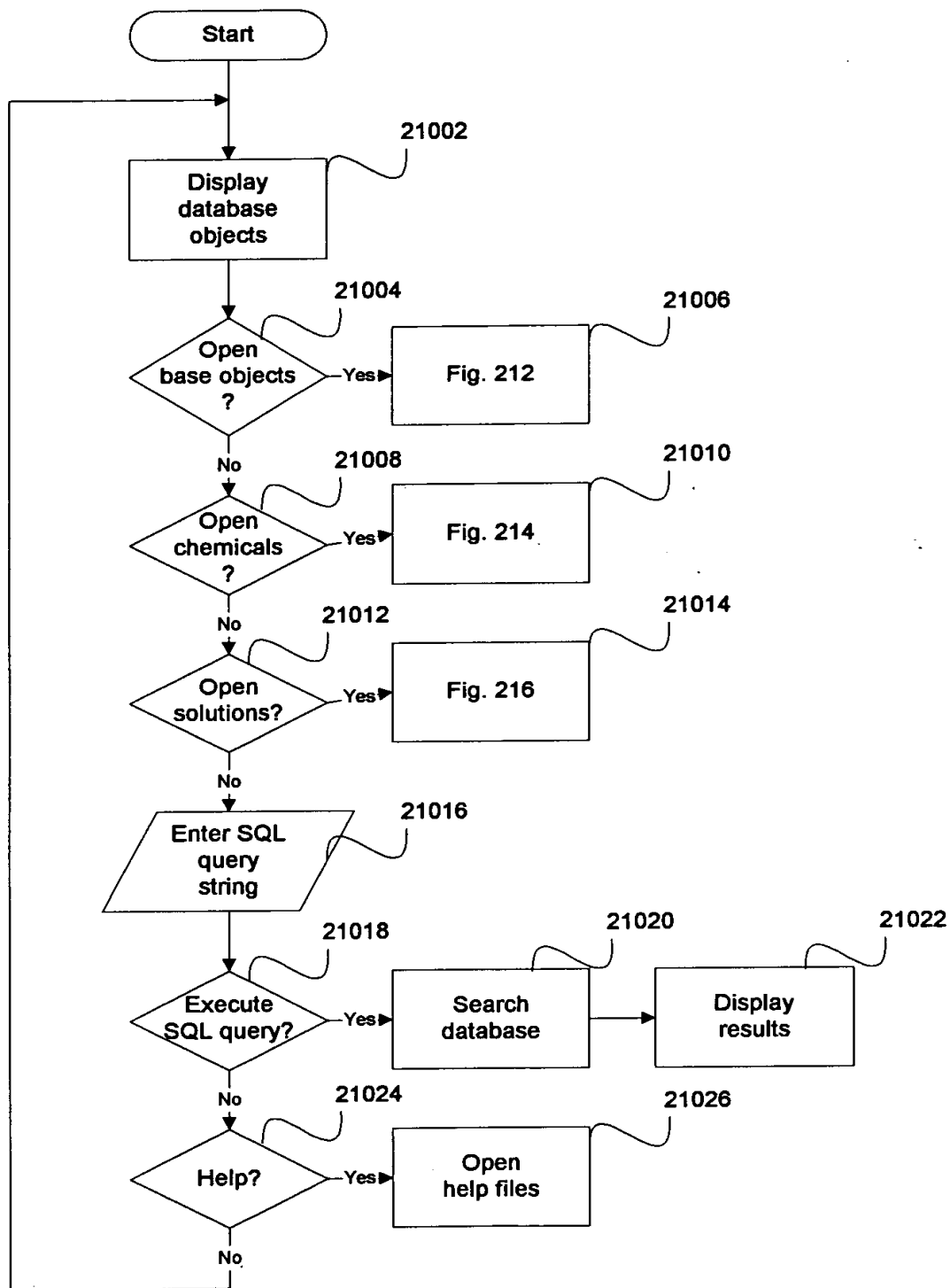


FIGURE 210



002080-587E96  
21106  
21112  
21101  
21108  
21110  
21102

Database Object Manager

Crystal Monitor Objects:

- Base Objects
- Chemicals
  - Buffering Agent
  - pHConjugate
  - Precipitant
  - Salt**
  - CSI
  - Chelator
  - Detergent
  - ReducingAgent
  - CryoCoolant
  - NucleationSuppressant
  - Organic
  - HeavyAtomCompound
  - Metal
  - Gas
  - Solvent
  - Other
- Solutions
- Data Mining

Attributes:

ChemicalName	ShortName	Formula	MolecularMass
dimethylarsinic ...	sodium cacodyl...	C2H6AsO2Na	160.
sodium citrate tri...	sodium citrate	C6H5Na3O7•2H...	294.1
ammonium sulfate	ammonium sulfate	(NH4)2SO4	132.1
ammonium sulfate	ammonium sulfate	(NH4)2SO4	132.1
ammonium sulfate	ammonium sulfate	(NH4)2SO4	132.1
lithium sulfate m...	lithium sulfate	Li2SO4•H2O	128.
ammonium phos...	dibasic ammoniu...	(NH4)2HPO4	132.1
sodium chloride	sodium chloride	NaCl	58.44
sodium phospho...	monobasic sodi...	NaH2PO4	120.
sodium phospho...	monobasic sodi...	NaH2PO4	120.
sodium phospho...	monobasic sodi...	NaH2PO4	119.96
potassium sodiu...	K/Na tartrate	C4H4O6NaK•4H...	282.2
sodium formate	sodium formate	CHO2Na	68.01
zinc acetate dihy...	zinc acetate	Zn(C2H3O2)2•2...	219.5
magnesium chlo...	magnesium chlo...	MgCl2•6H2O	203.3
calcium acetate	calcium acetate	Ca(C2H3O2)2	158.2
magnesium acet...	magnesium acet...	Mg(C2H3O2)2•4...	214.5

Execute SQL Query

26 rows. Query time: 411 ms

Help

21100

21102

21104

Fig. 211



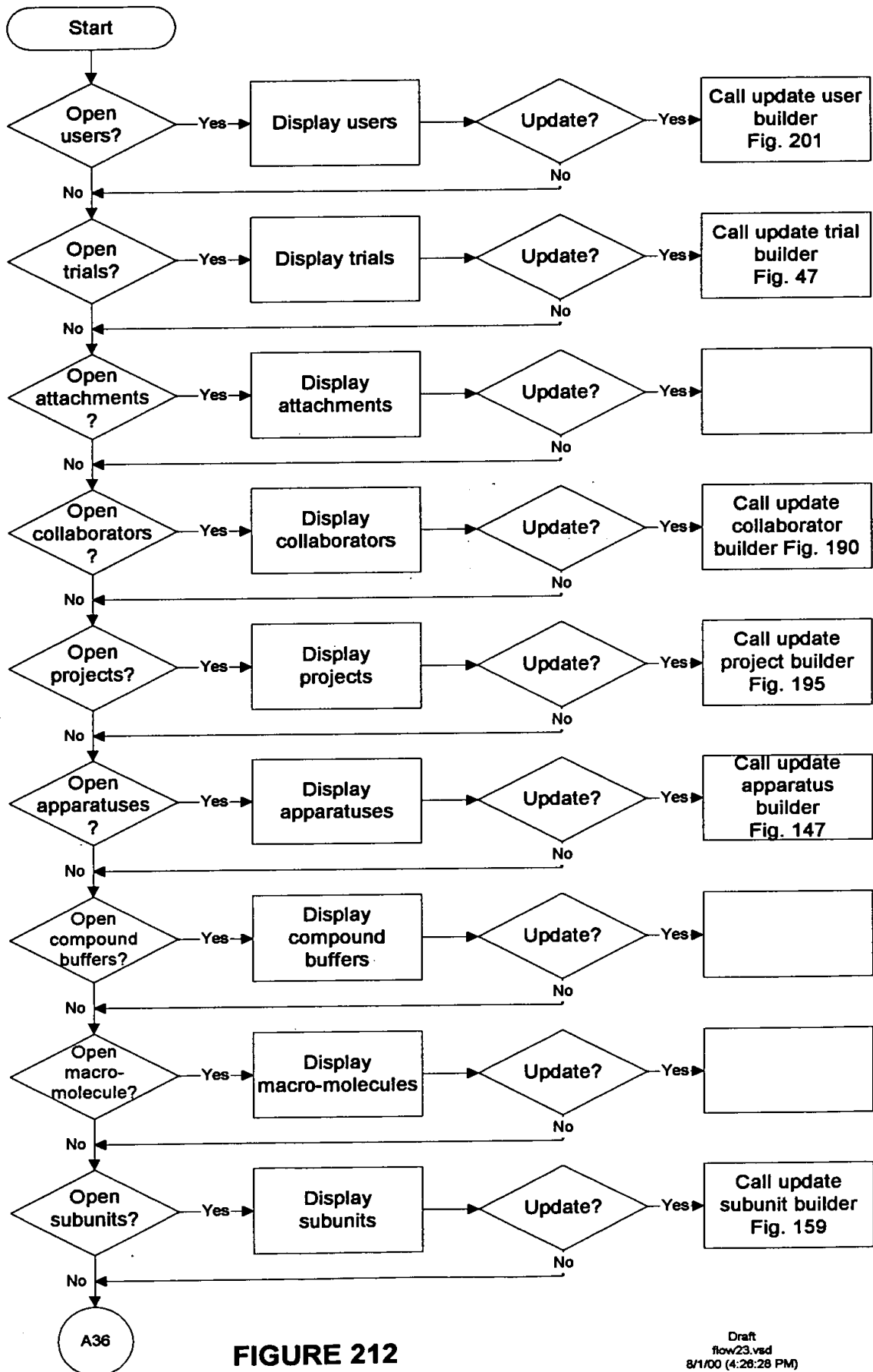


FIGURE 212

002000" 58T'E960

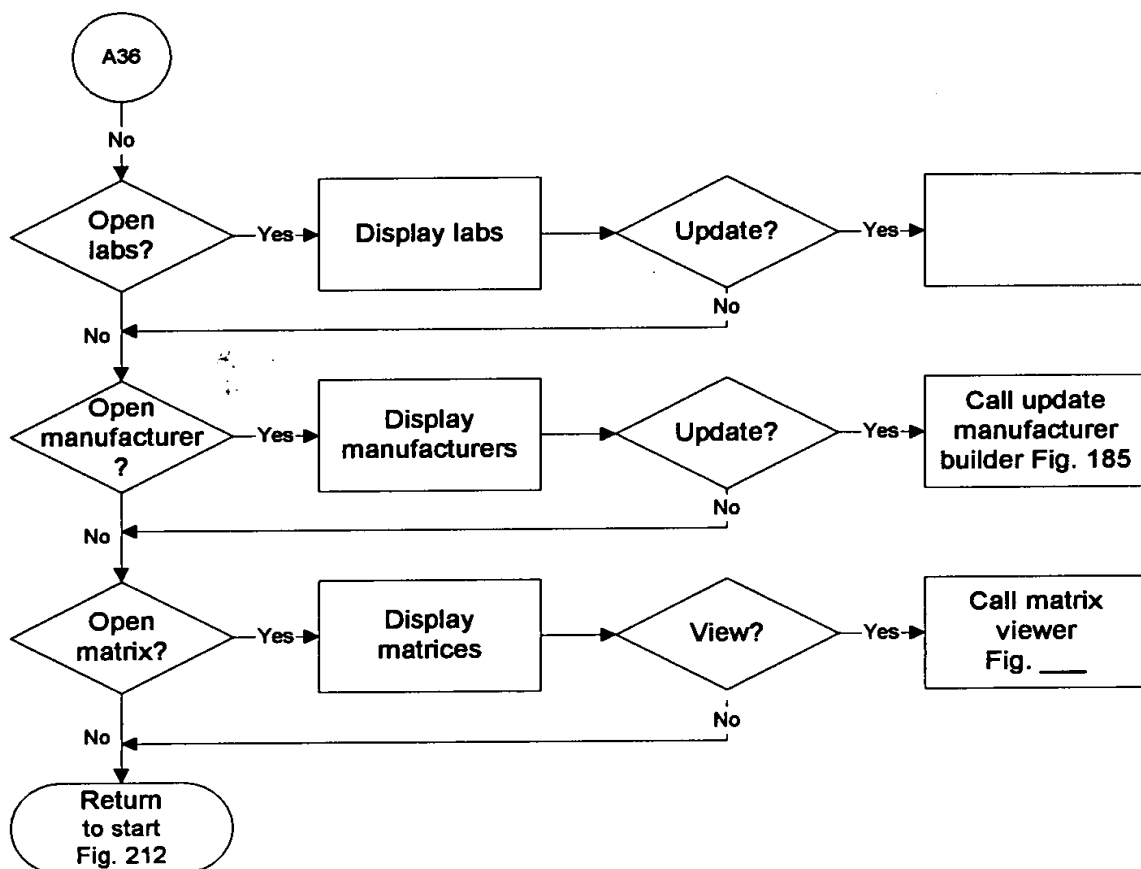


FIGURE 213

002080" 5317E960

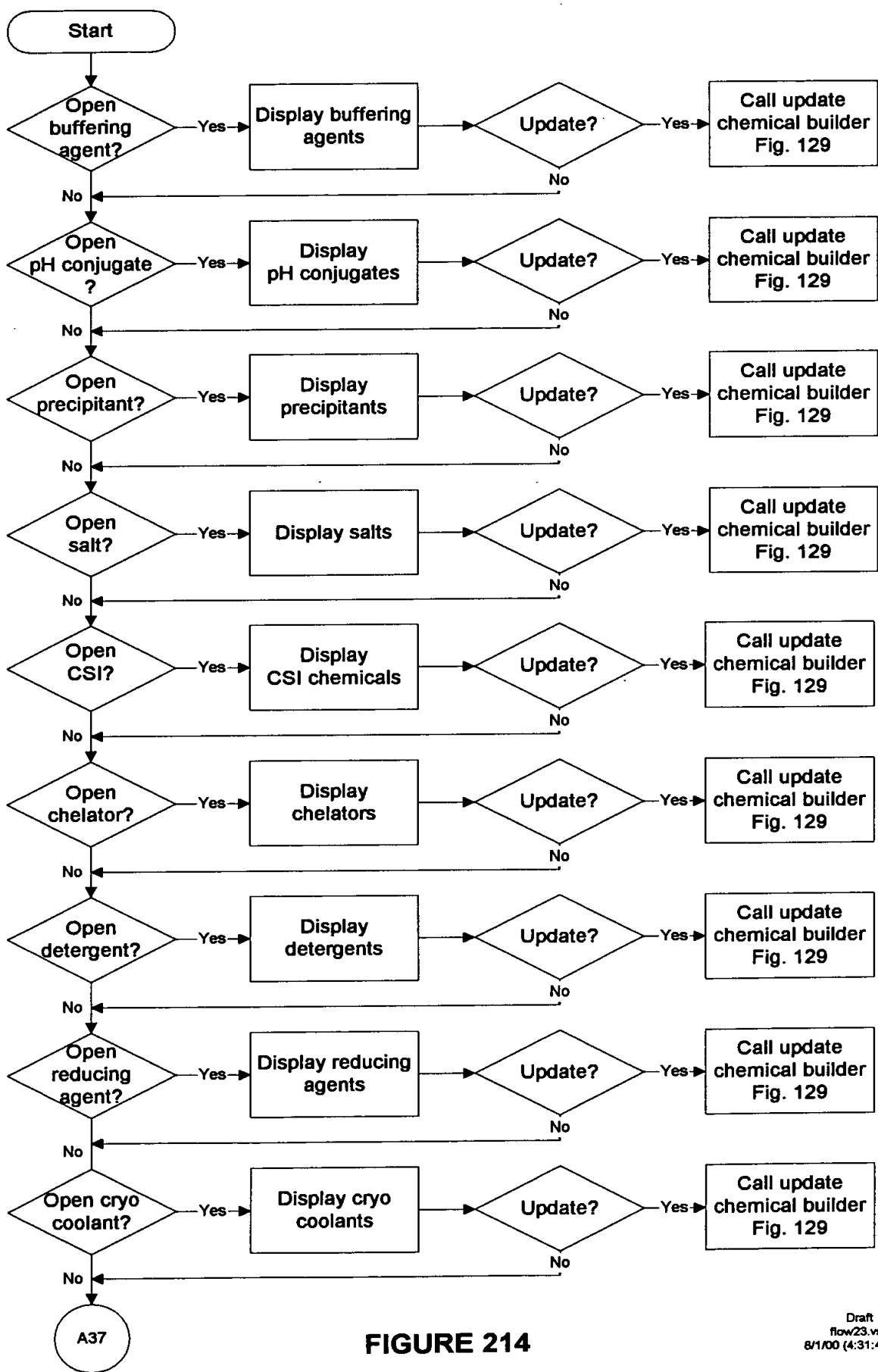


FIGURE 214

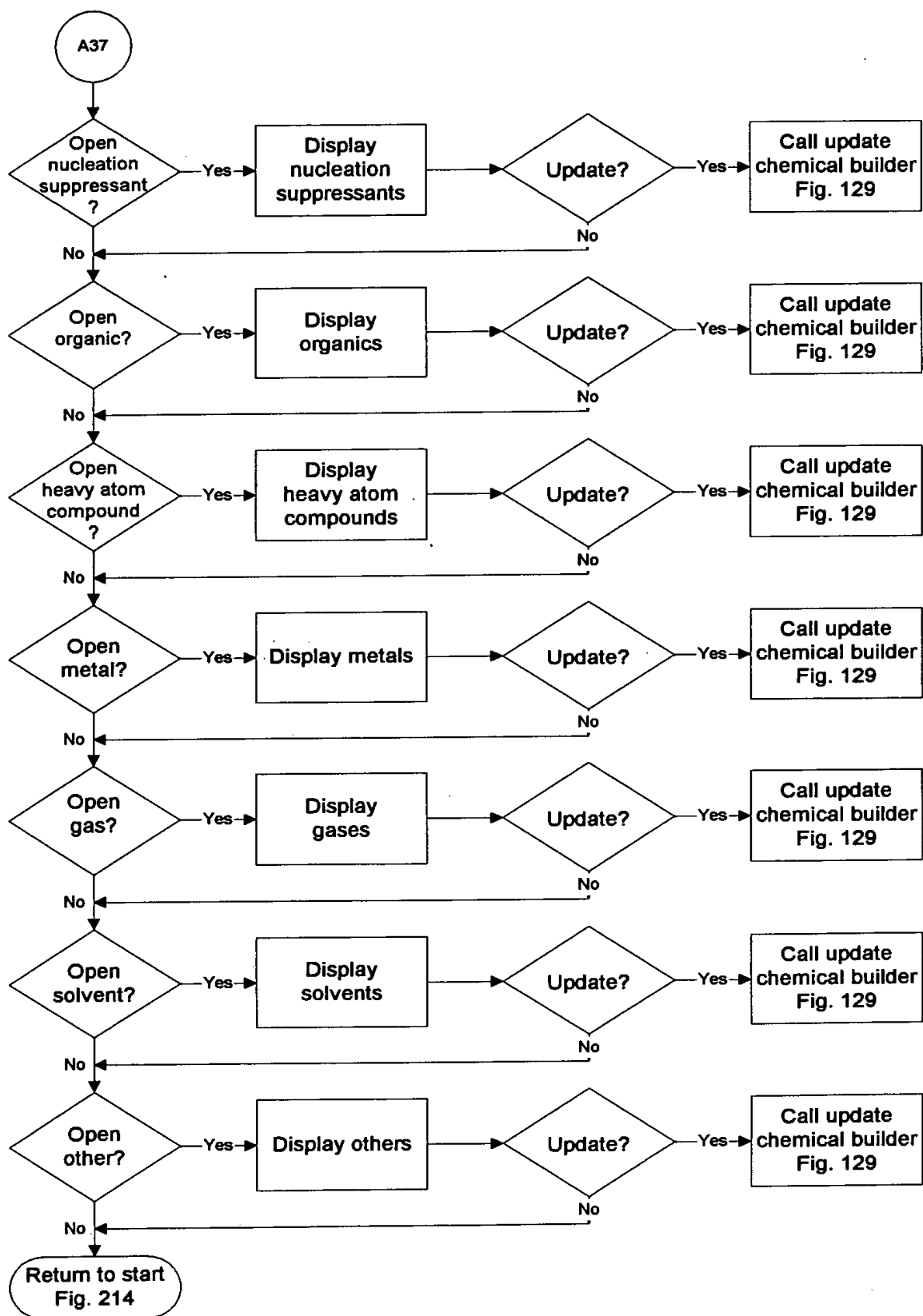


FIGURE 215

002080"58T.E.960

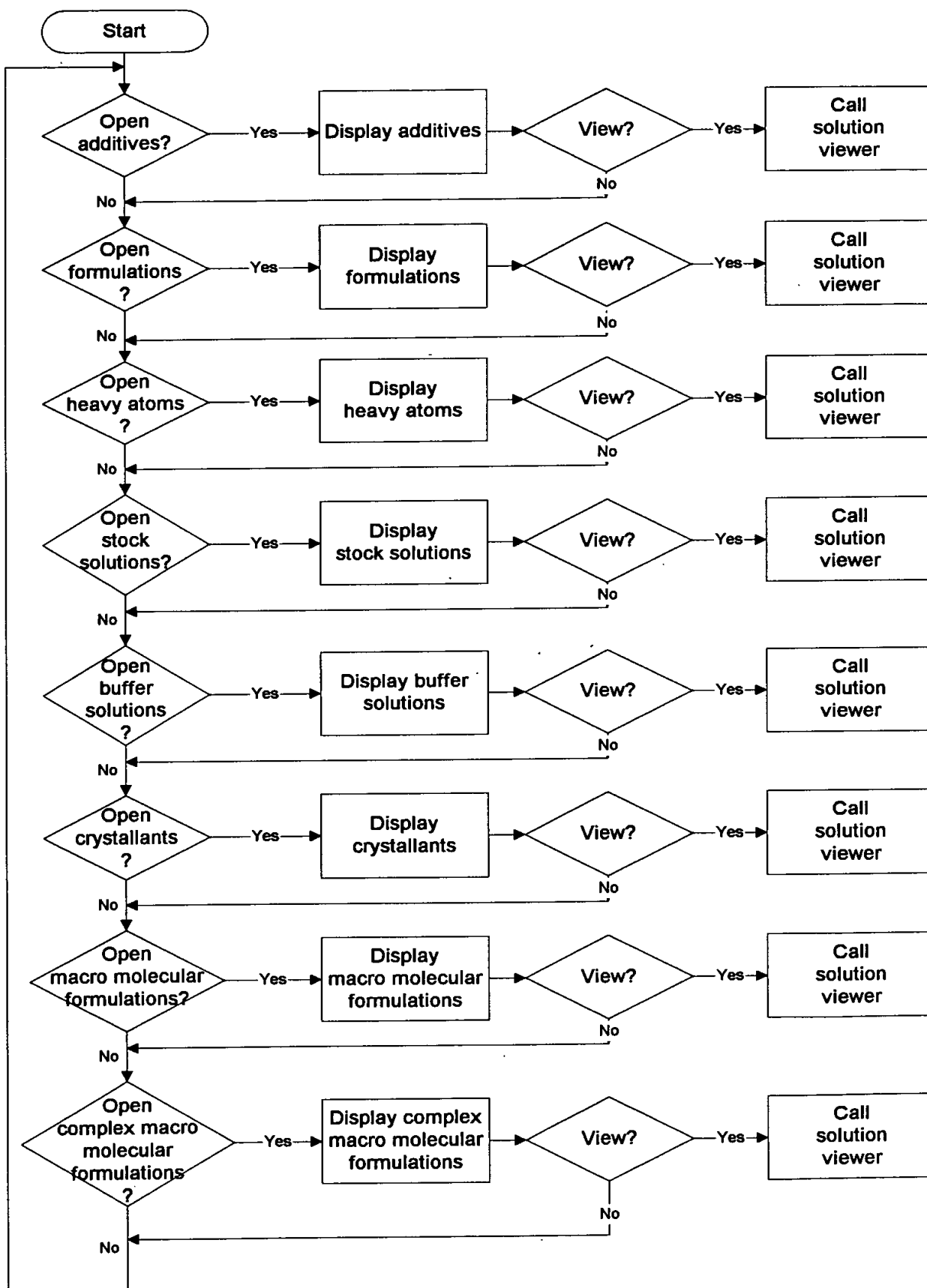


FIGURE 216

002080"587TE960

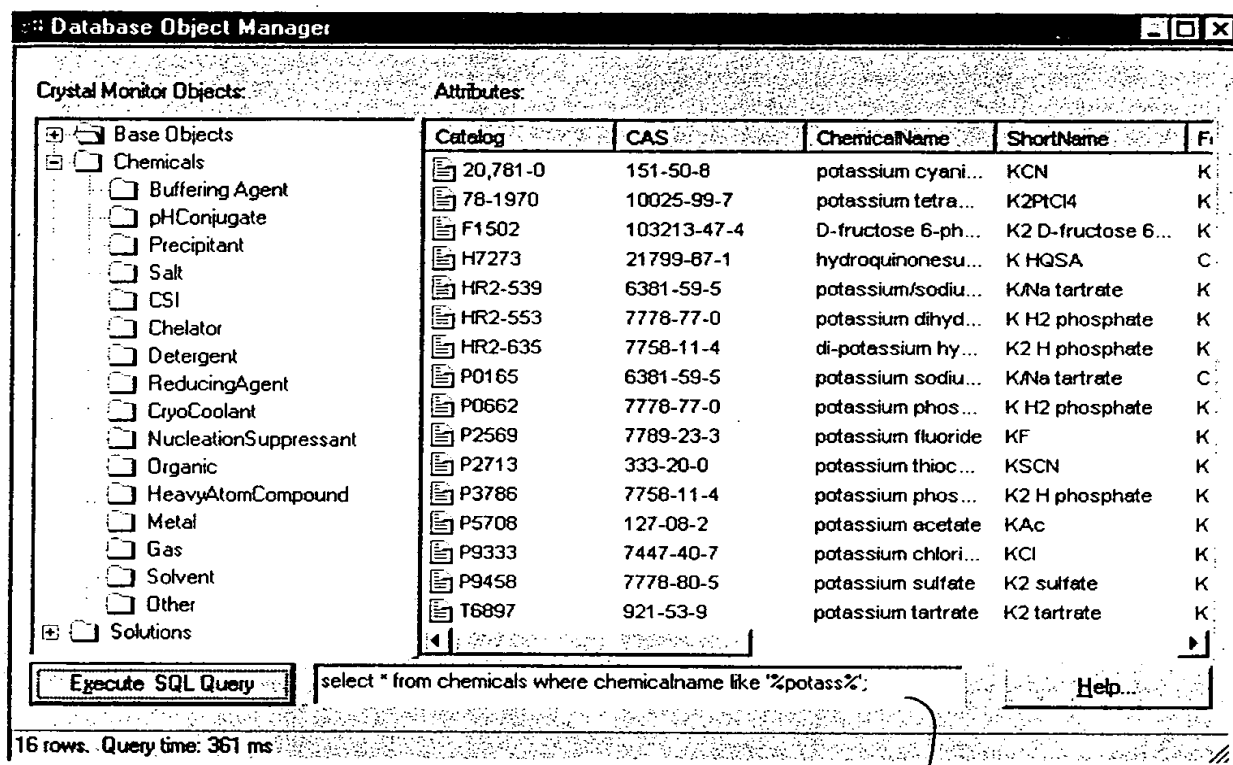


Fig. 217

21700

002080" 587E960

Database Object Manager

Crystal Monitor Objects:

- Base Objects
- Chemicals
  - Buffering Agent
  - pHConjugate
  - Precipitant
  - Salt
  - CSI
  - Chelator
  - Detergent
  - ReducingAgent
  - CryoCoolant
  - NucleationSuppressant
  - Organic
  - HeavyAtomCompound
  - Metal
  - Gas
  - Solvent
  - Other
- Solutions

Attributes:

Catalog	CAS	ChemicalName	ShortName
A7330	631-61-8	ammonium acet...	NH4 Ac
HR2-565	631-61-8	ammonium acet...	NH4 Ac
A6141	1066-33-7	ammonium bicar...	NH4 bicarbonate
A5666	12125-02-9	ammonium chlori...	NH4 chloride
HR2-555	7722-76-1	ammonium dihyd...	NH4 H2 phosph...
F2004	540-69-2	ammonium form...	NH3 formate
A7455	6484-52-2	ammonium nitrate	NH4 nitrate
A1167	7783-28-0	ammonium phos...	(NH4)2 H phosph...
A2939	7783-20-2	ammonium sulfate	(NH4)2 sulfate
A938-500	7783-20-2	ammonium sulfate	(NH4)2 sulfate
HR2-541	7783-20-2	ammonium sulfate	(NH4)2 sulfate
JT0792-5	7783-20-2	ammonium sulfate	(NH4)2 sulfate
B6394	10326-27-9	barium chloride ...	Ba chloride
C4705	62-54-4	calcium acetate	CaAc2
HR2-567	62-54-4	calcium acetate	CaAc2
C5080	10035-04-8	calcium chloride...	CaCl2

Execute SQL Query

Help...

77 rows. Query time: 81 ms

21800

Fig. 218

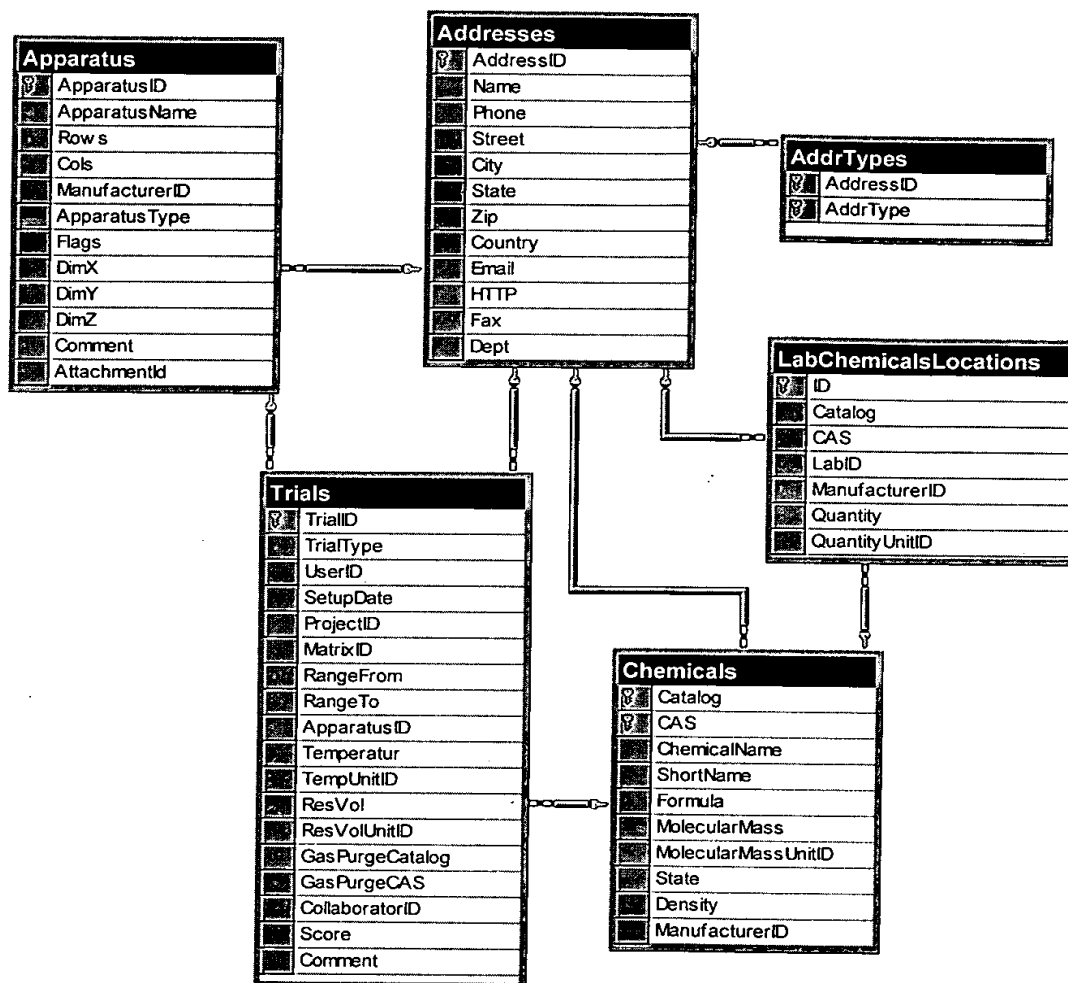
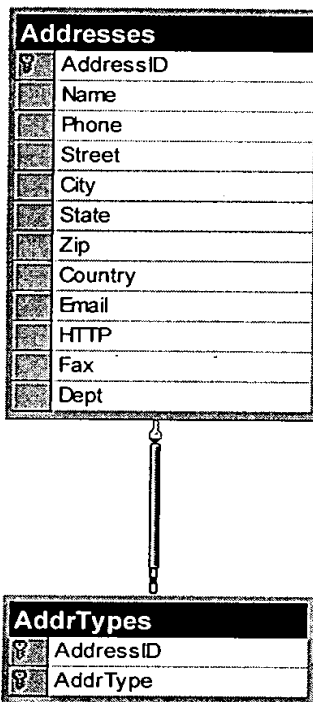


Fig. 219





**Fig. 220**

002080-587E960

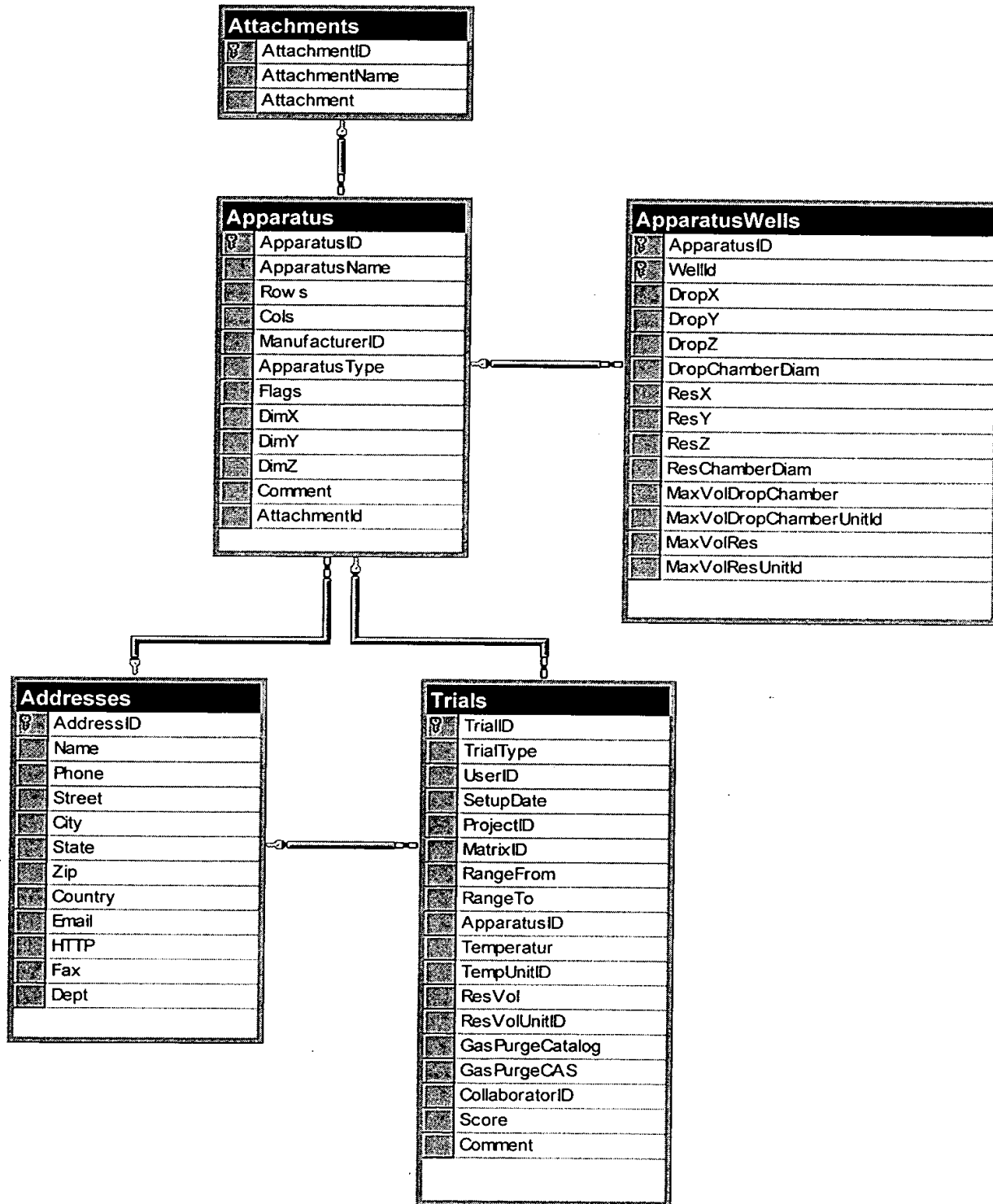
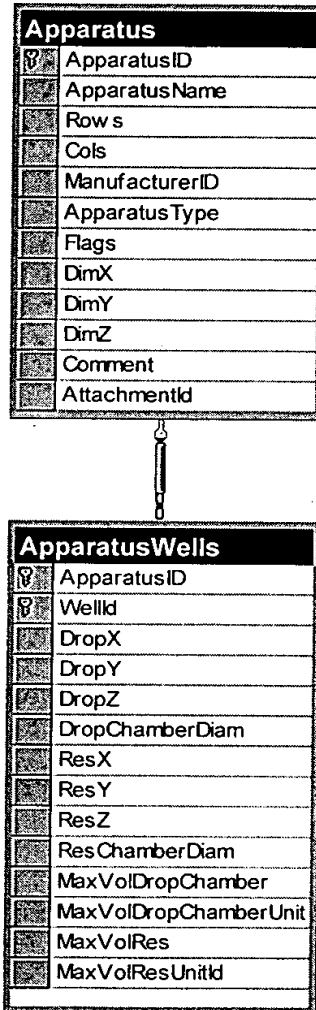


Fig. 221

002080\*58T2960



**Fig. 222**

002080"587E960

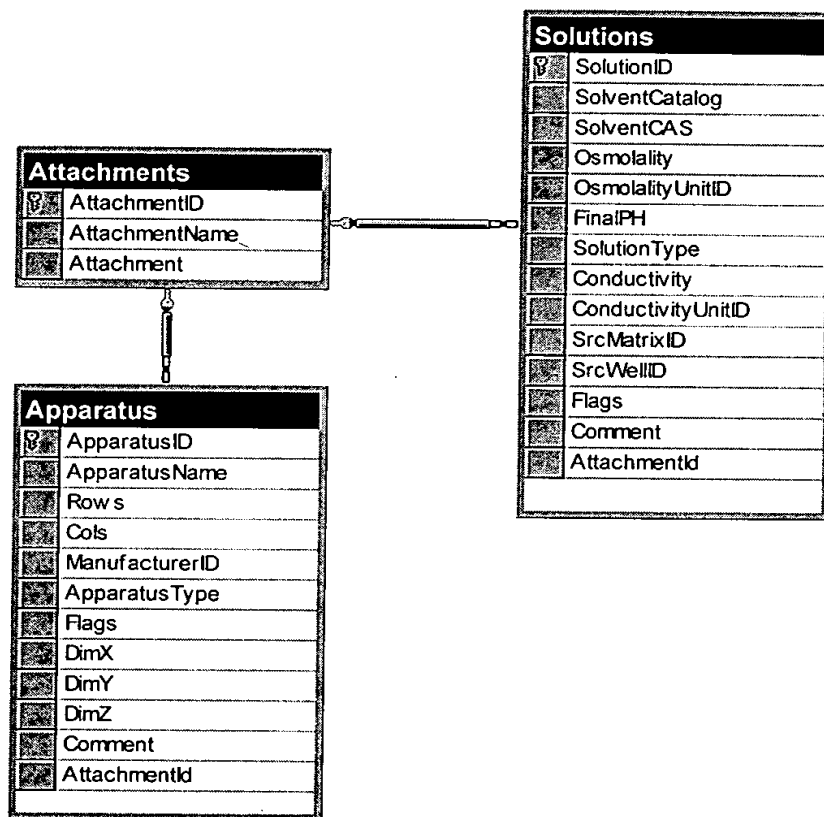


Fig. 223

002080" 58T E960

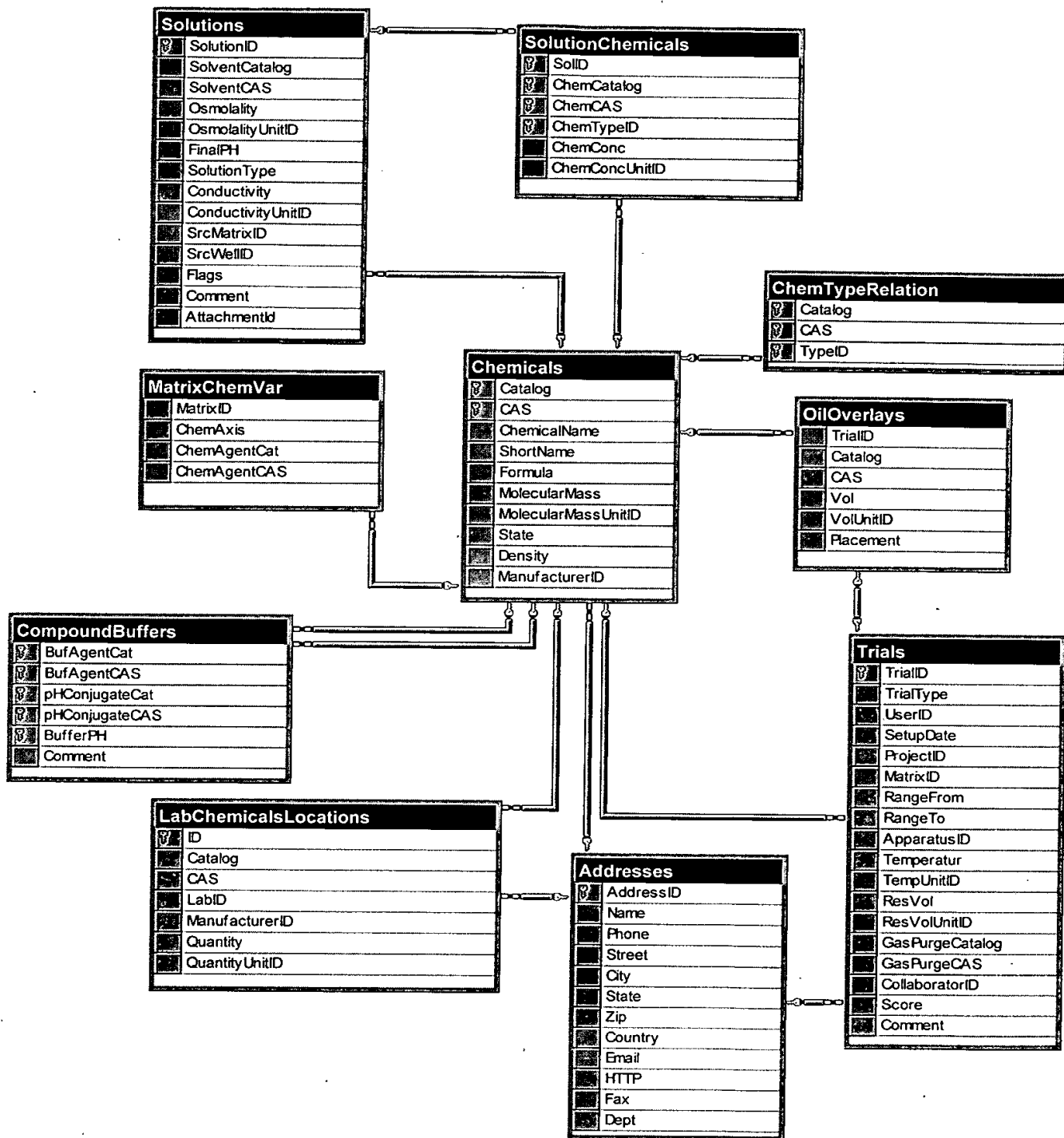


Fig. 224

002080 " 55T E960

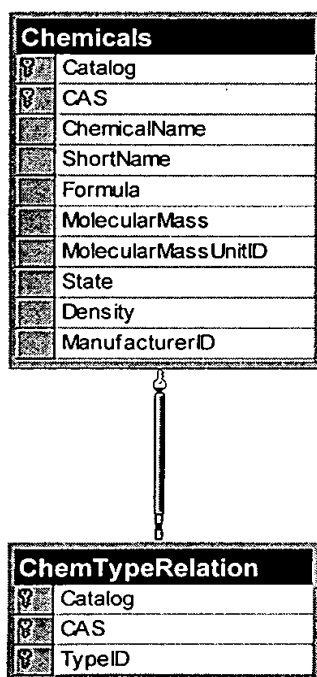


Fig. 225

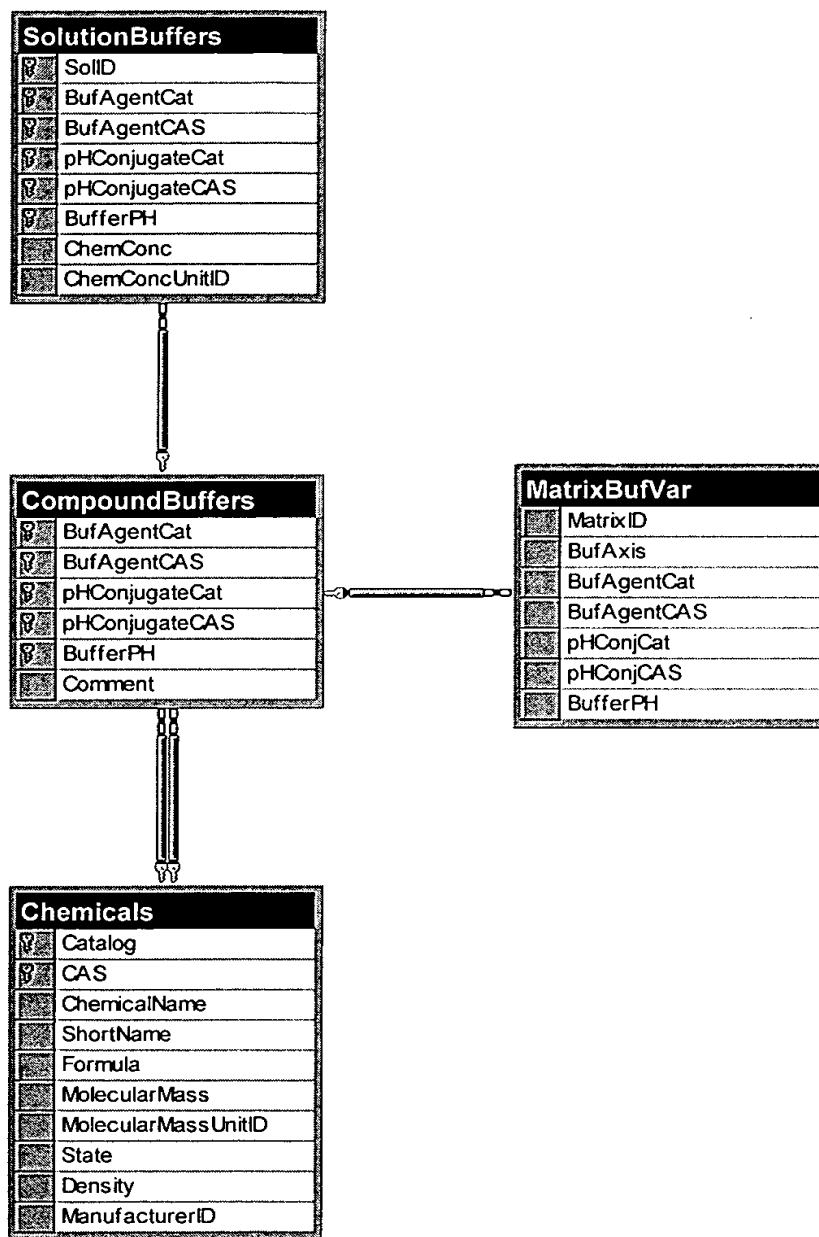


Fig. 226

002080" 58T9960

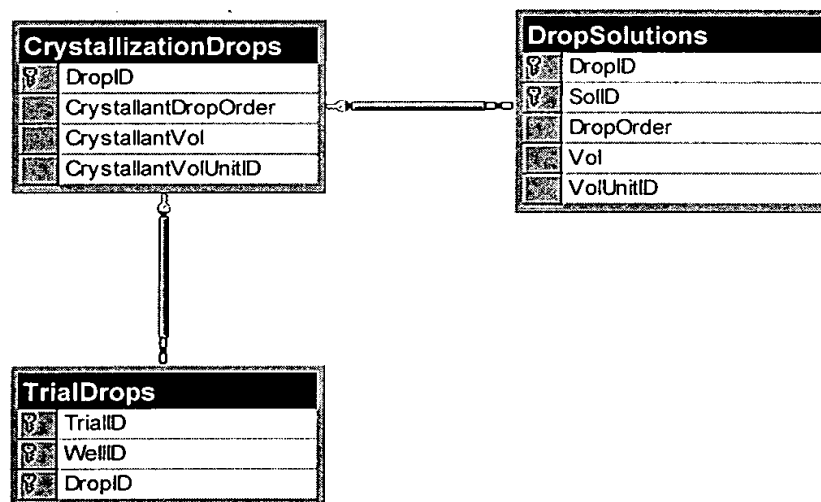
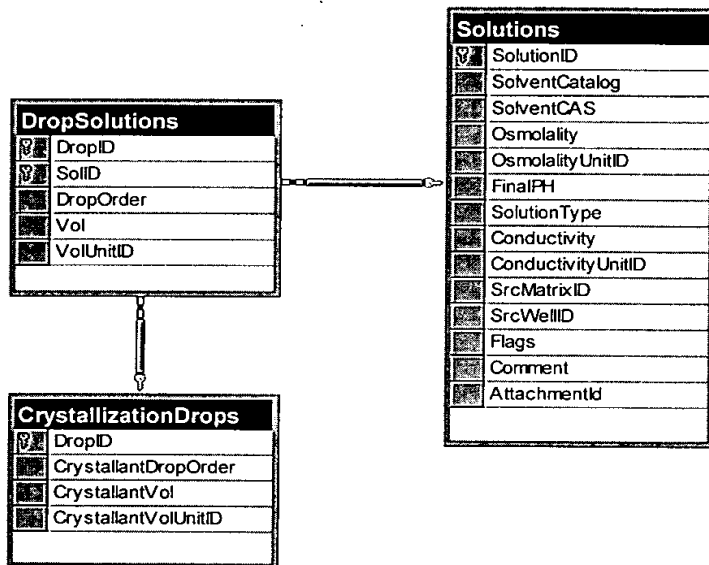


Fig. 227





**Fig. 228**

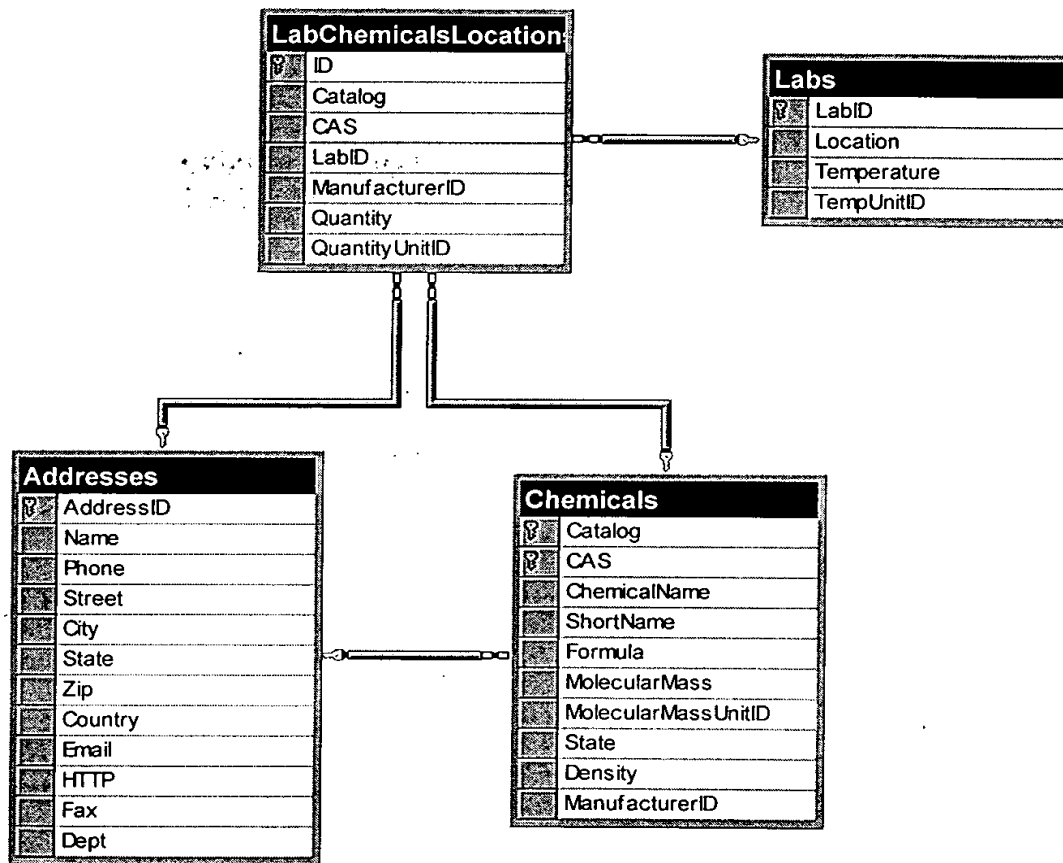
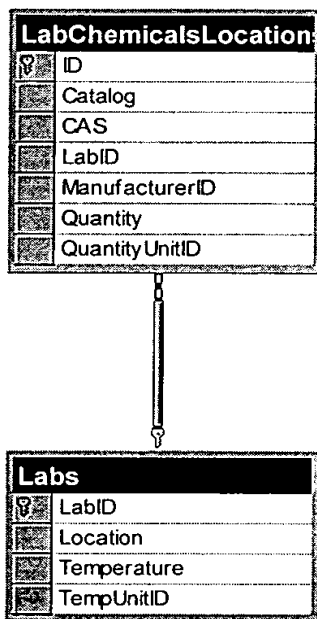


Fig. 229

002020" SSTFE960



**Fig. 230**

002020-587590

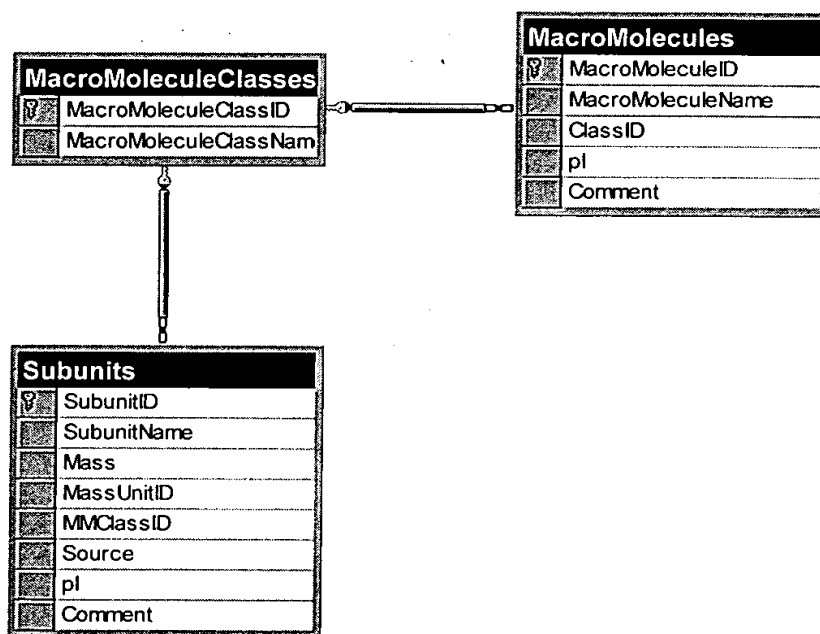
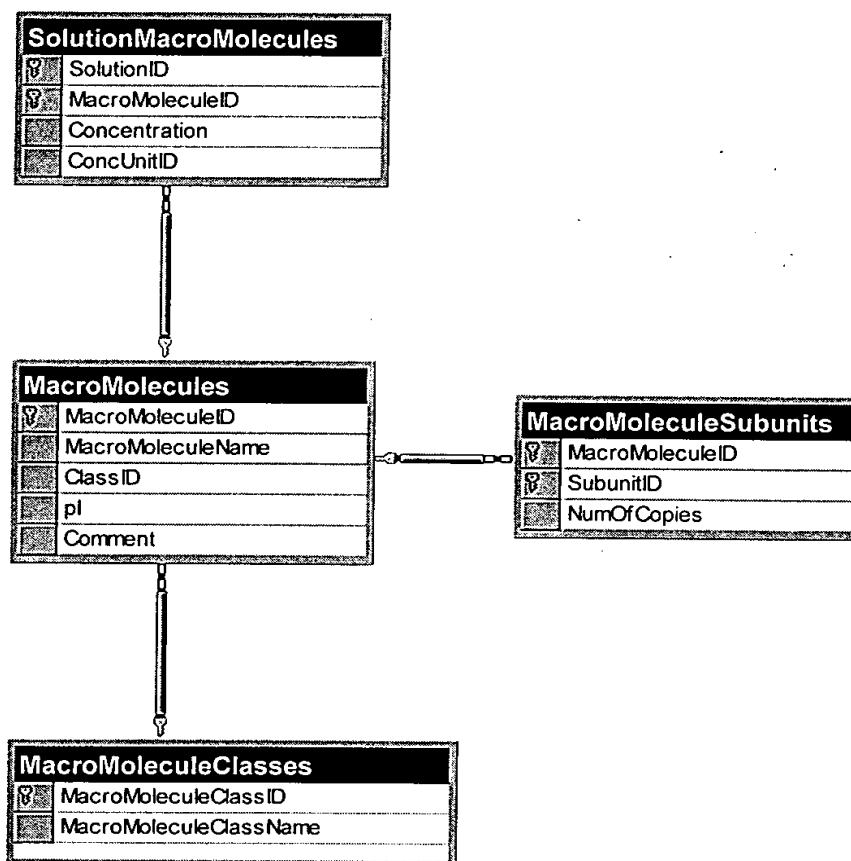


Fig. 231

002080" 59TTE960



**Fig. 232**

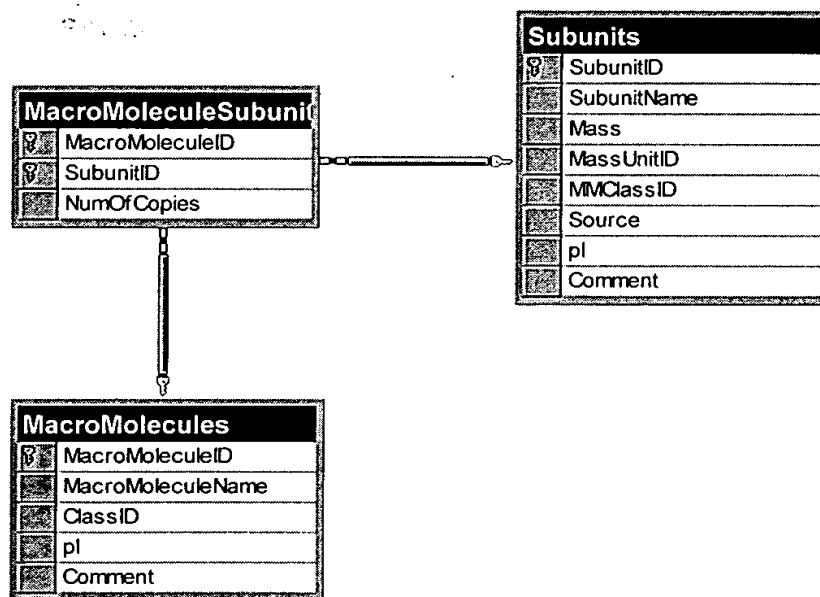


Fig. 233

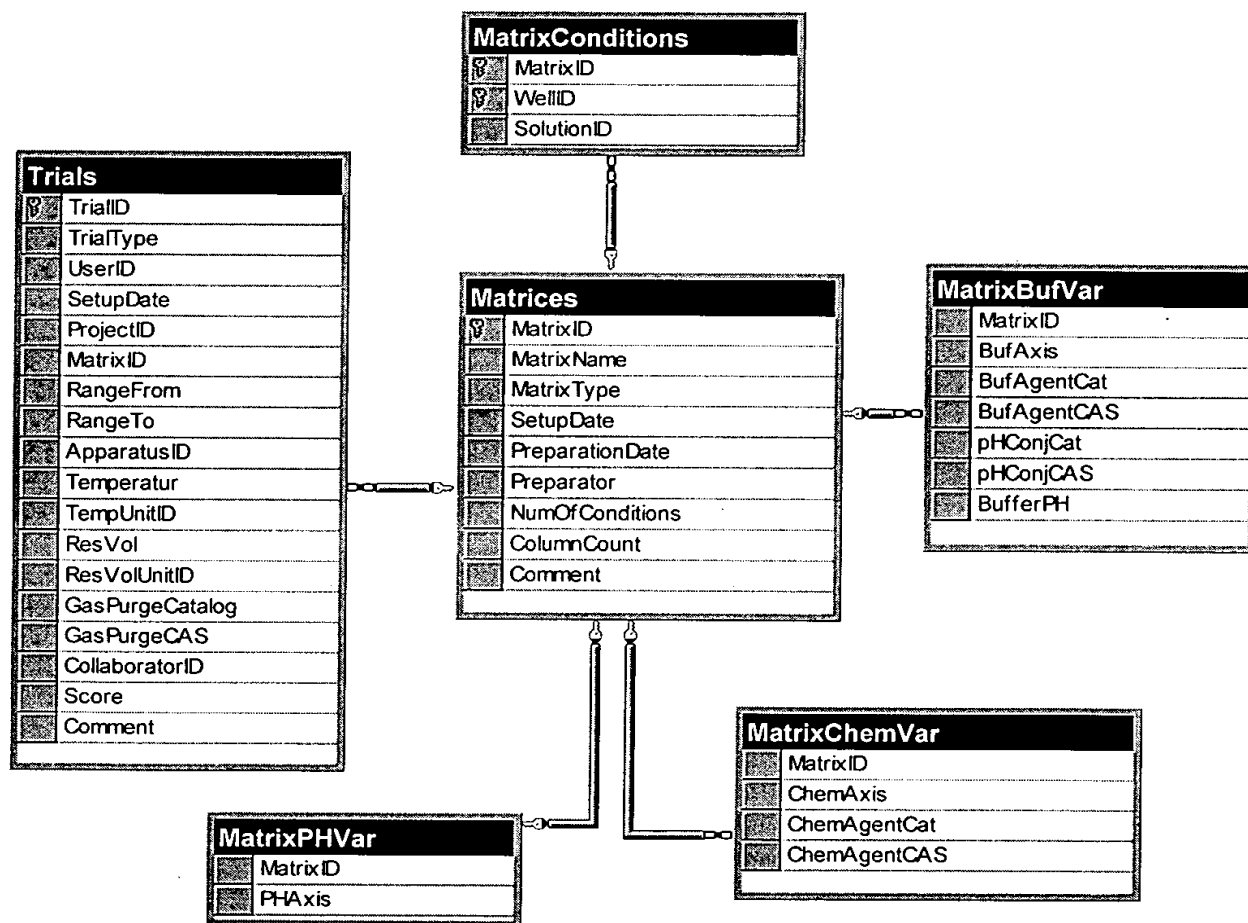
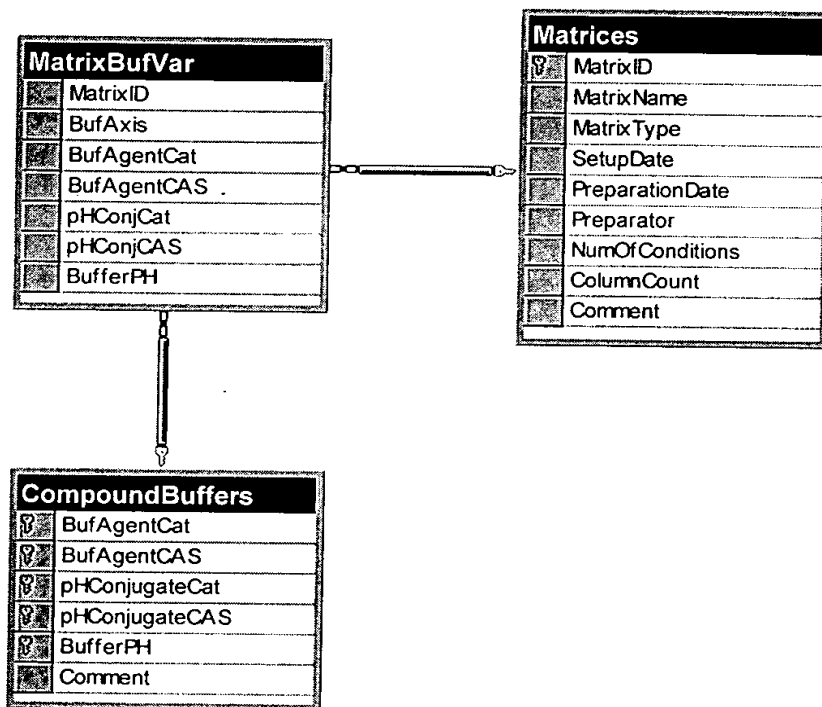


Fig. 234

002080"58T960



**Fig. 235**



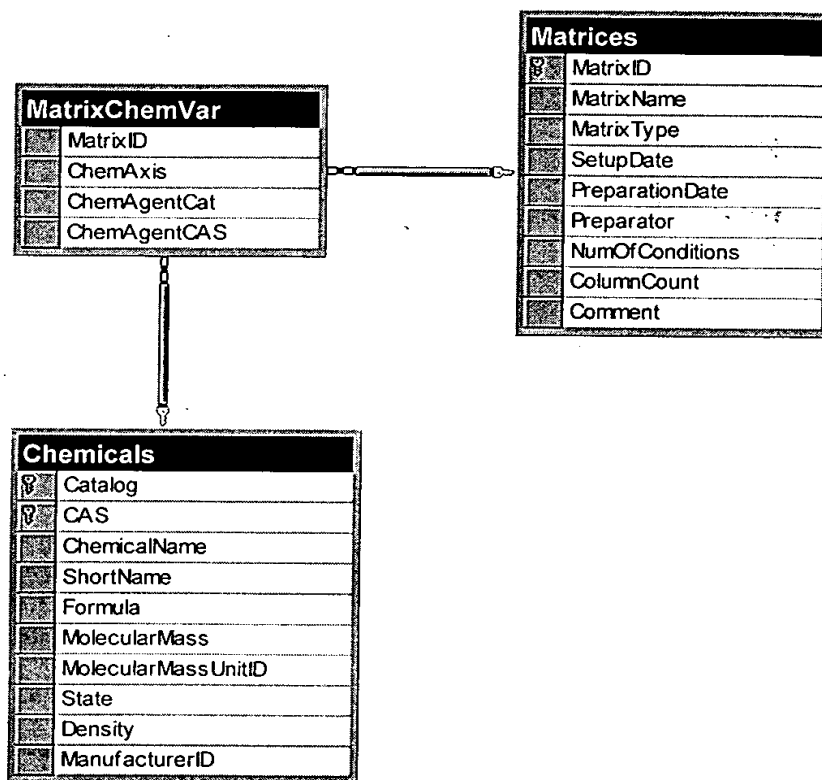


Fig. 236

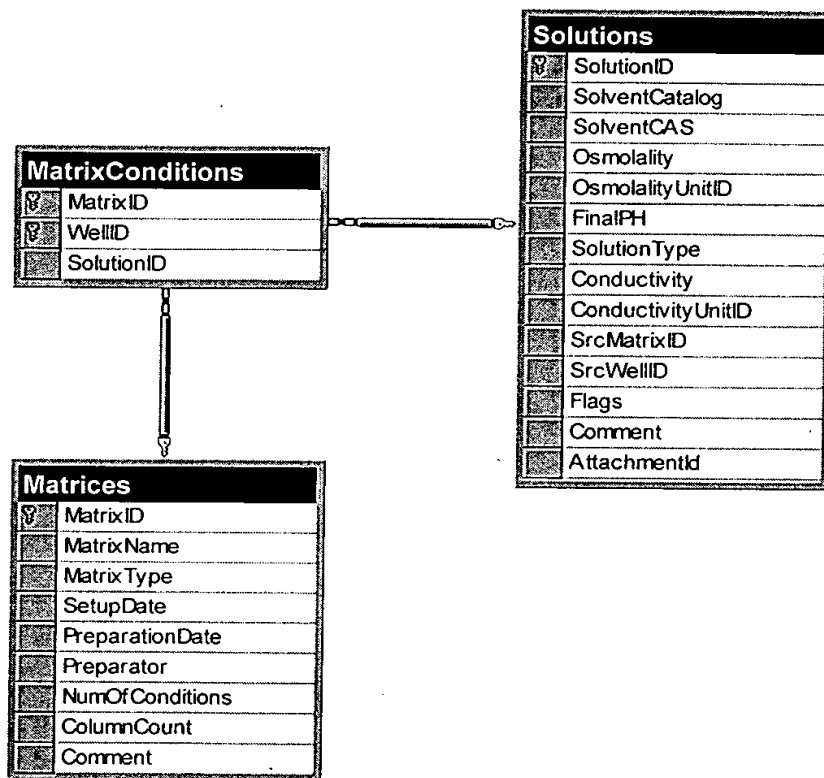
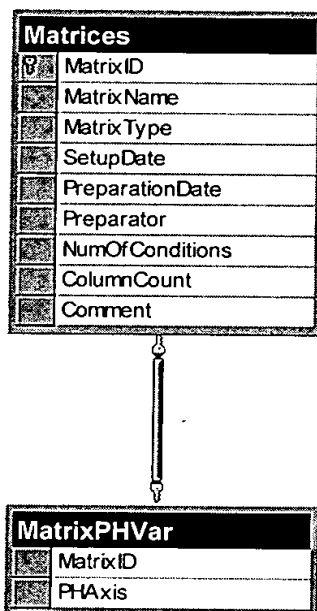
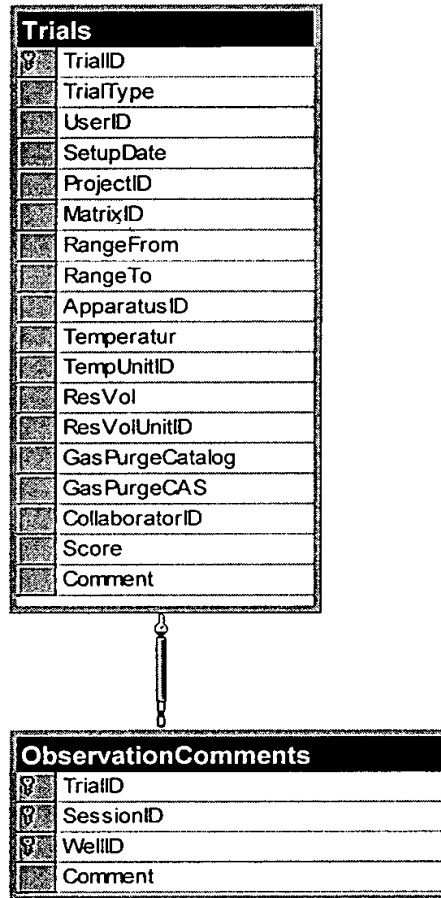


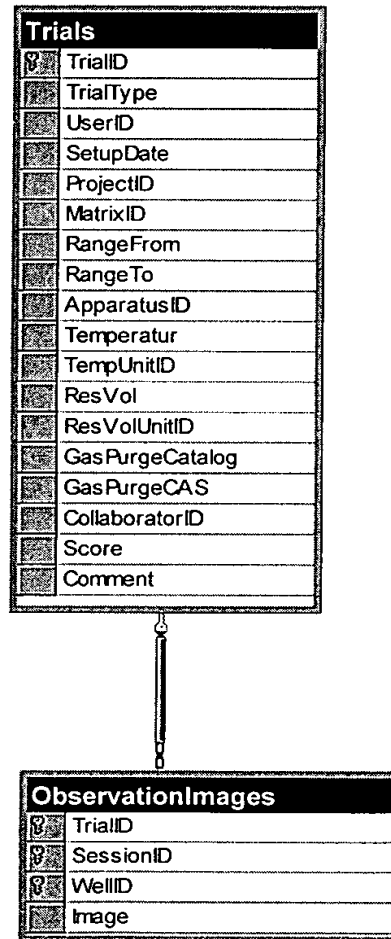
Fig. 237

**Fig. 238**

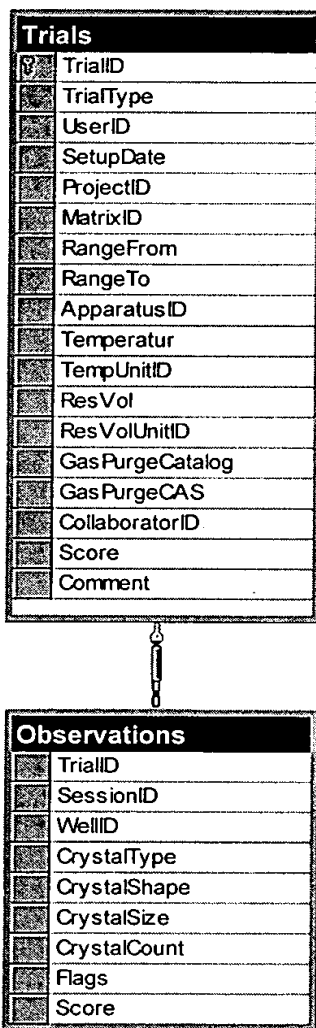
002080-5877E960



**Fig. 239**

**Fig. 240**

002030"58T1E960



**Fig. 241**

002030" 58TF360

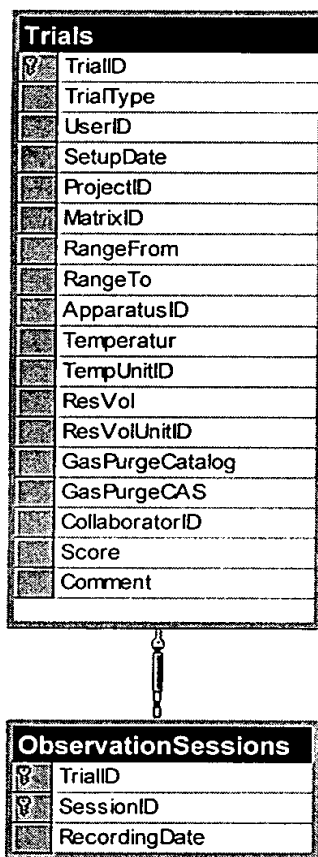


Fig. 242

002080" SST12960

Trials	
<input checked="" type="checkbox"/>	TrialID
<input type="checkbox"/>	TrialType
<input type="checkbox"/>	UserID
<input type="checkbox"/>	SetupDate
<input type="checkbox"/>	ProjectID
<input type="checkbox"/>	MatrixID
<input type="checkbox"/>	RangeFrom
<input type="checkbox"/>	RangeTo
<input type="checkbox"/>	ApparatusID
<input type="checkbox"/>	Temperatur
<input type="checkbox"/>	TempUnitID
<input type="checkbox"/>	ResVol
<input type="checkbox"/>	ResVolUnitID
<input type="checkbox"/>	GasPurgeCatalog
<input type="checkbox"/>	GasPurgeCAS
<input type="checkbox"/>	CollaboratorID
<input type="checkbox"/>	Score
<input type="checkbox"/>	Comment



ObservationWaveFiles	
<input checked="" type="checkbox"/>	TrialID
<input checked="" type="checkbox"/>	SessionID
<input checked="" type="checkbox"/>	WellID
<input type="checkbox"/>	WaveFile

Fig. 243



002080" 581E960

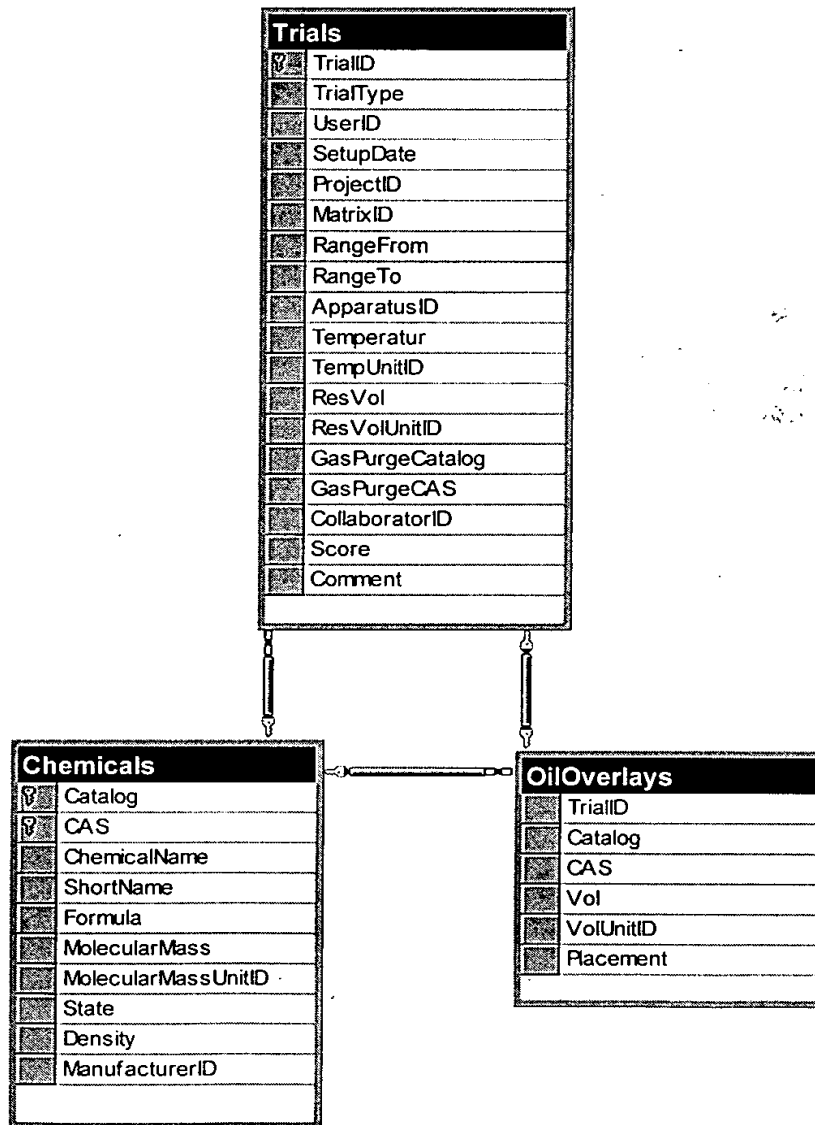




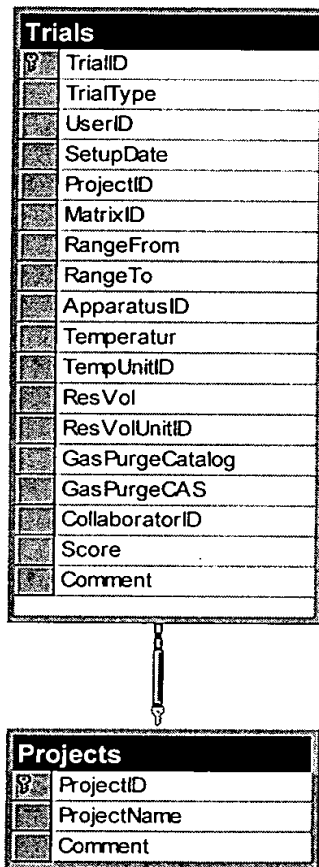
Fig. 244

002080" 58T'E960

Preparators	
	PreparatorID
	PreparatorName

**Fig. 245**

002030-587E960



**Fig. 246**

002080"597E96

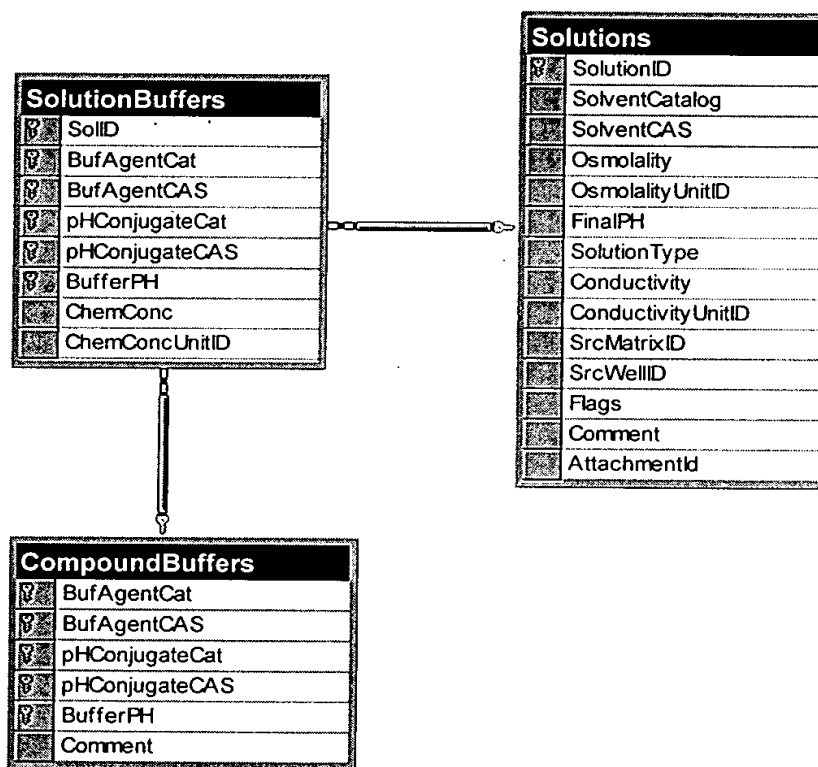


Fig. 247

002080"587E960

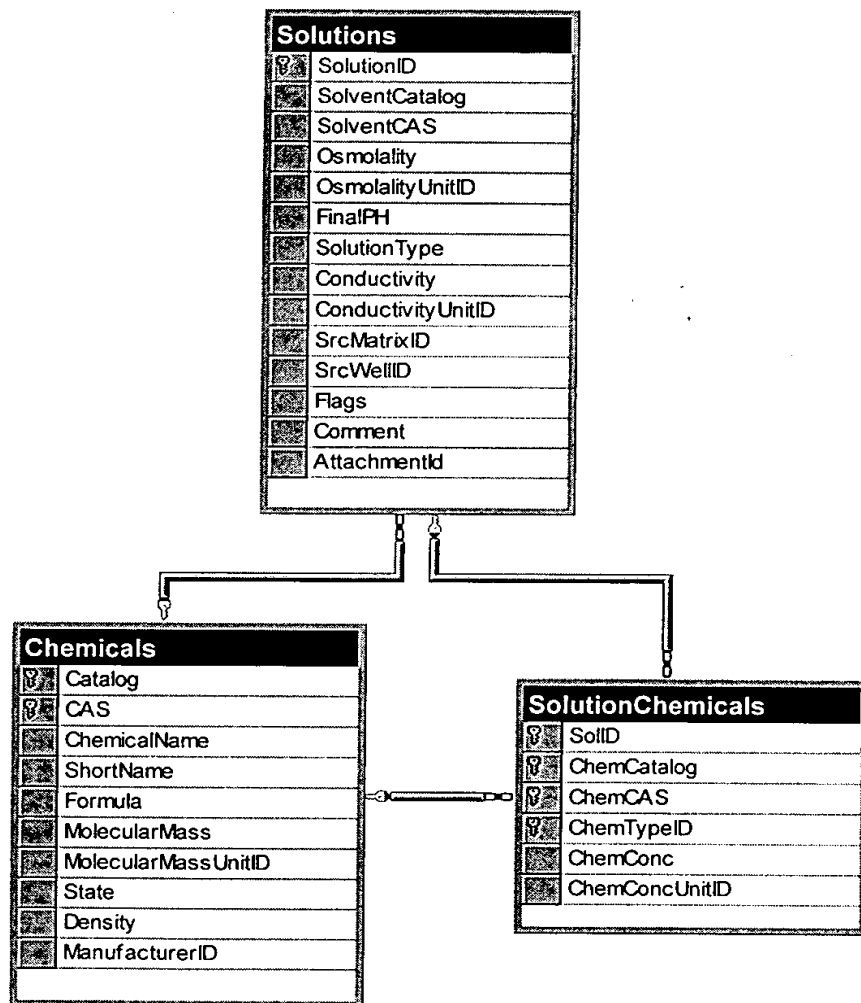


Fig. 248

002080'58T'960

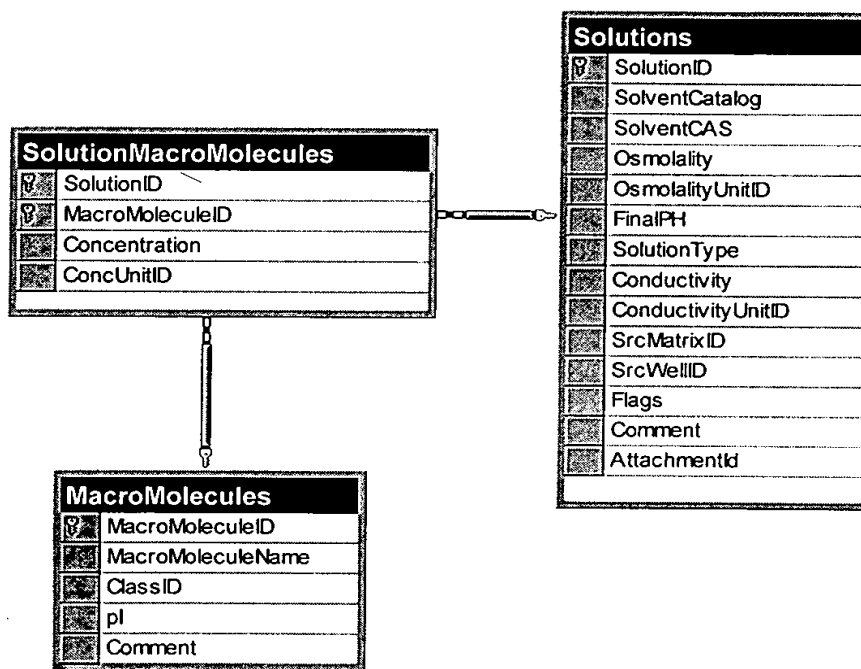


Fig. 249

002080"58TFE960

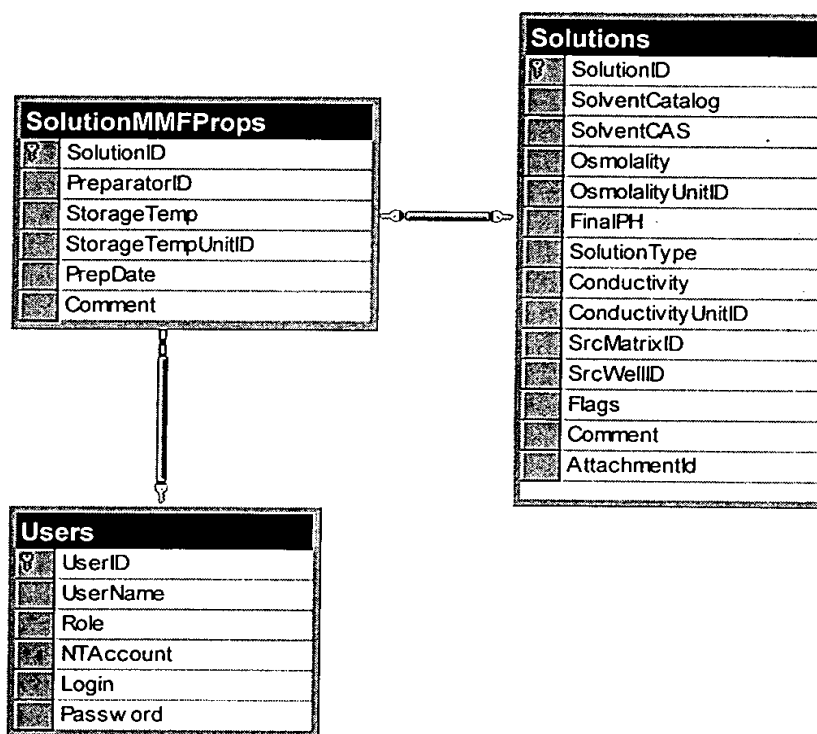
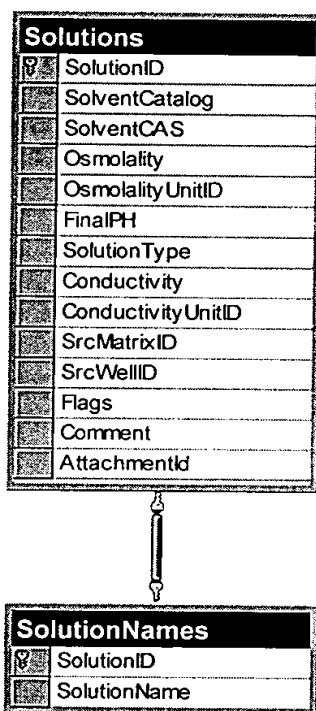


Fig. 250

002080"58TTE960



**Fig. 251**



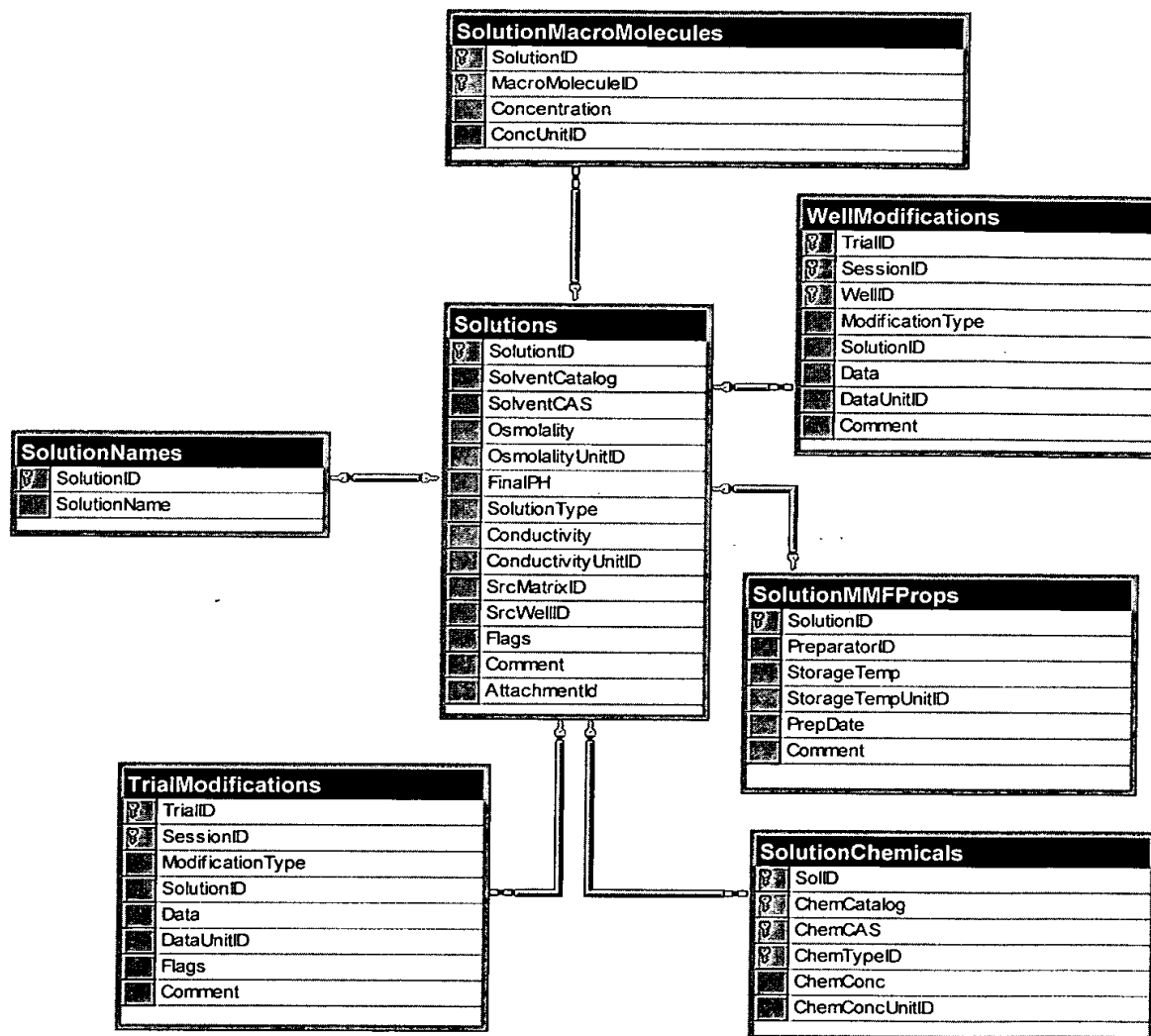


Fig. 252

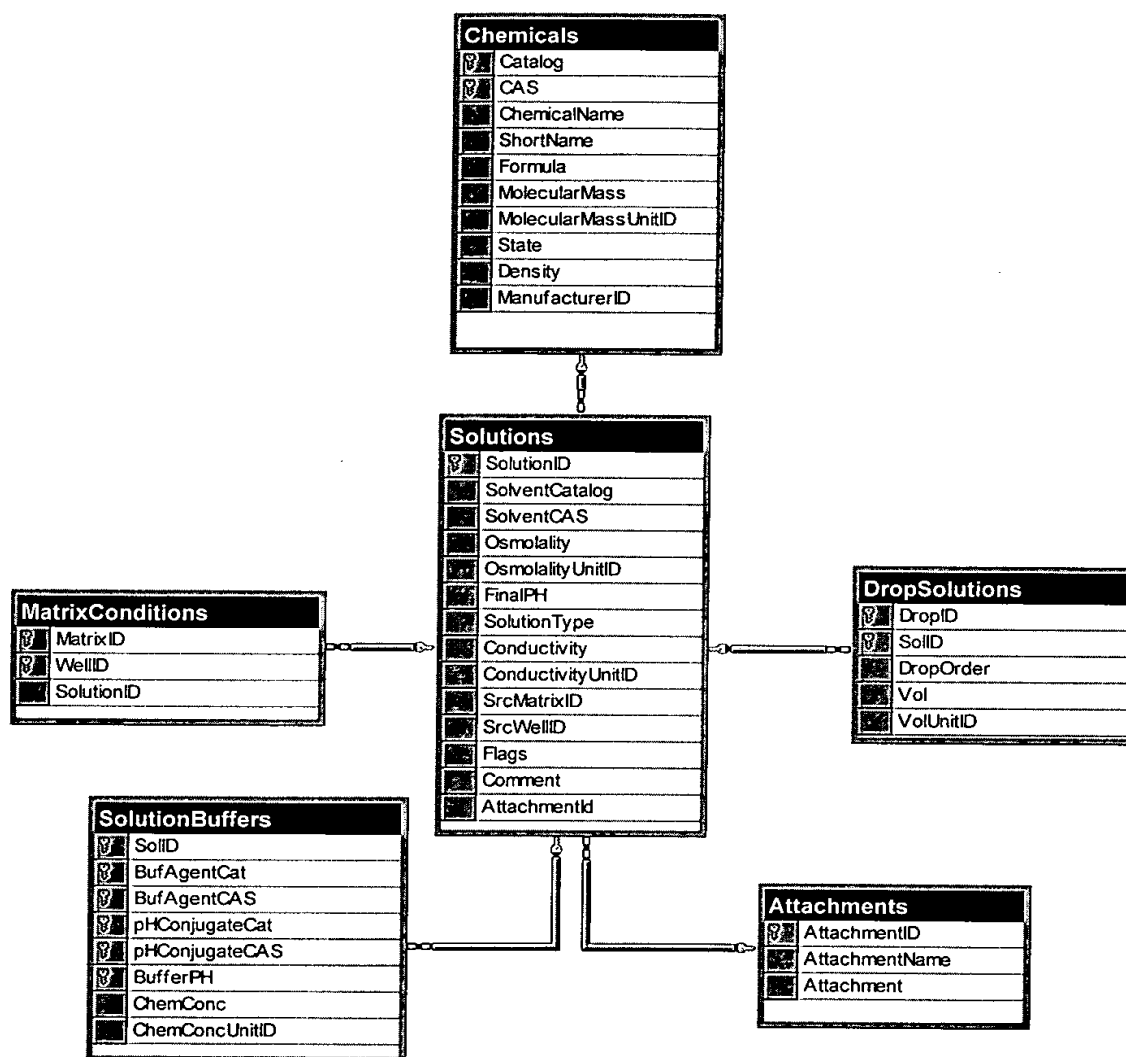


Fig. 253

002030" 58712960

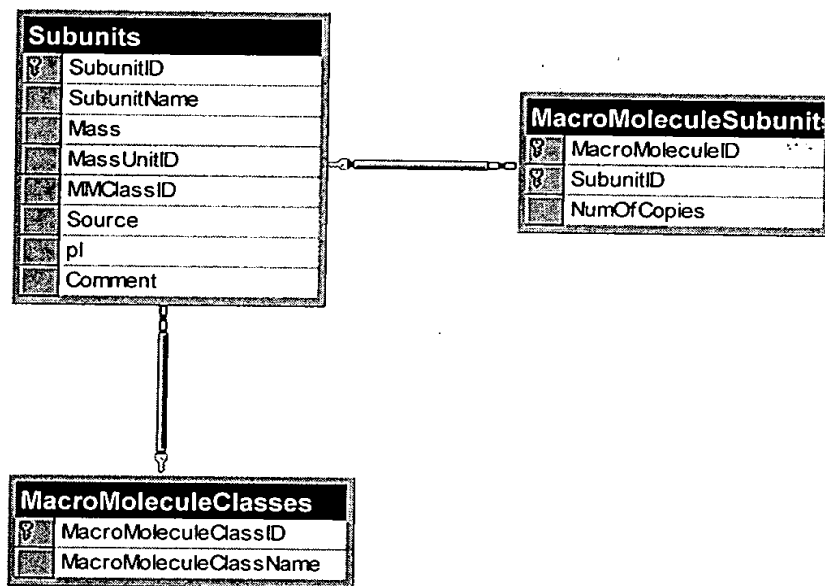


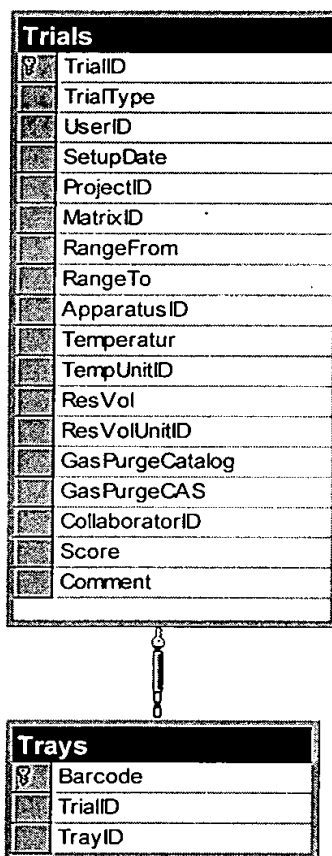
Fig. 254

002080" 58TE960

SystemInfo	
Attrib	
Value	

**Fig. 255**

002080"59T'E960



**Fig. 256**

002080" 58T E960

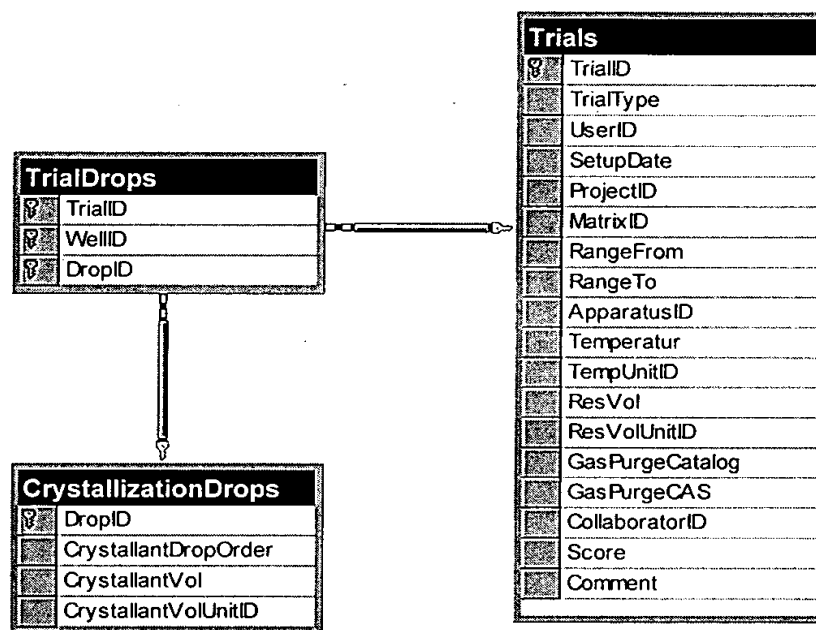


Fig. 257

0963185-030200

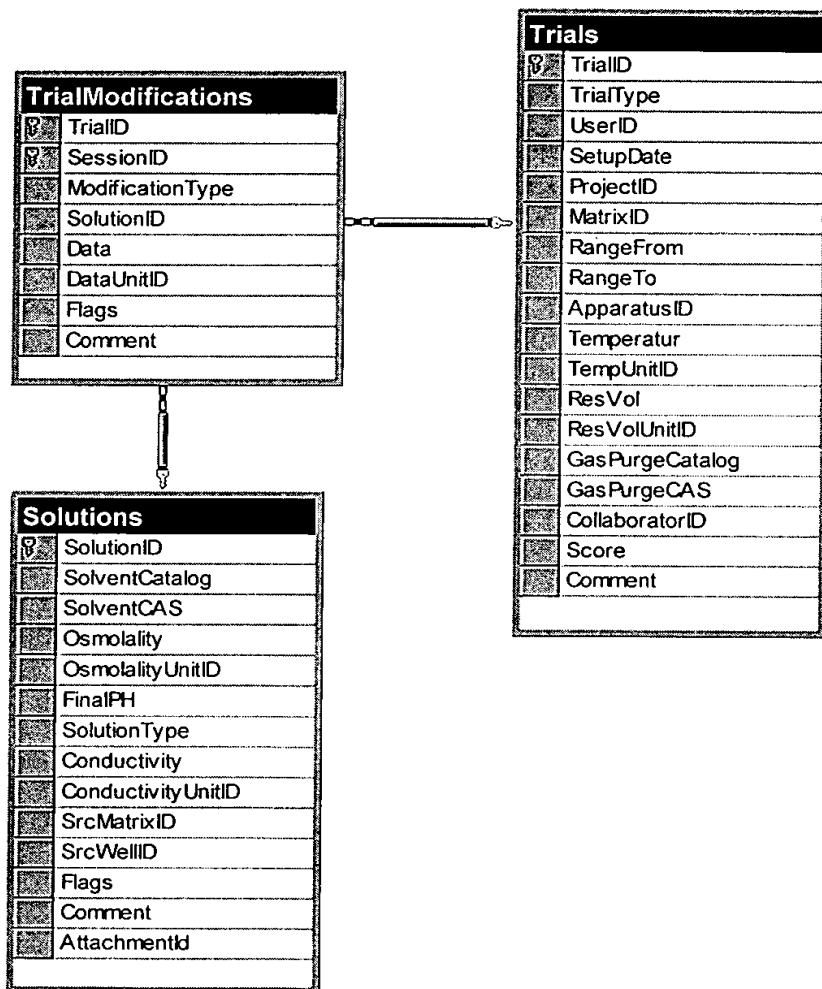


Fig. 258

002030 557E960

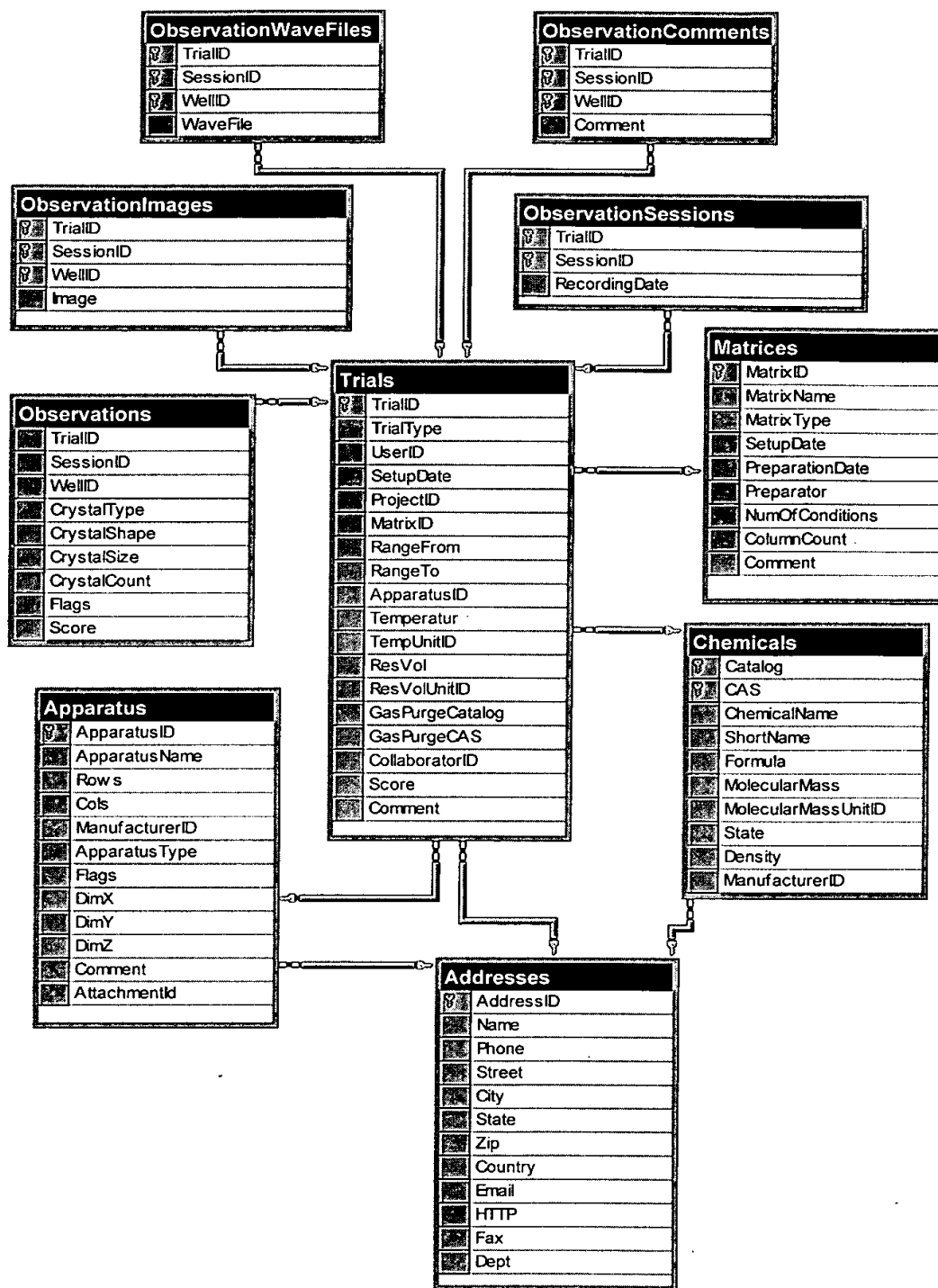


Fig. 259



002080" 58TCE960

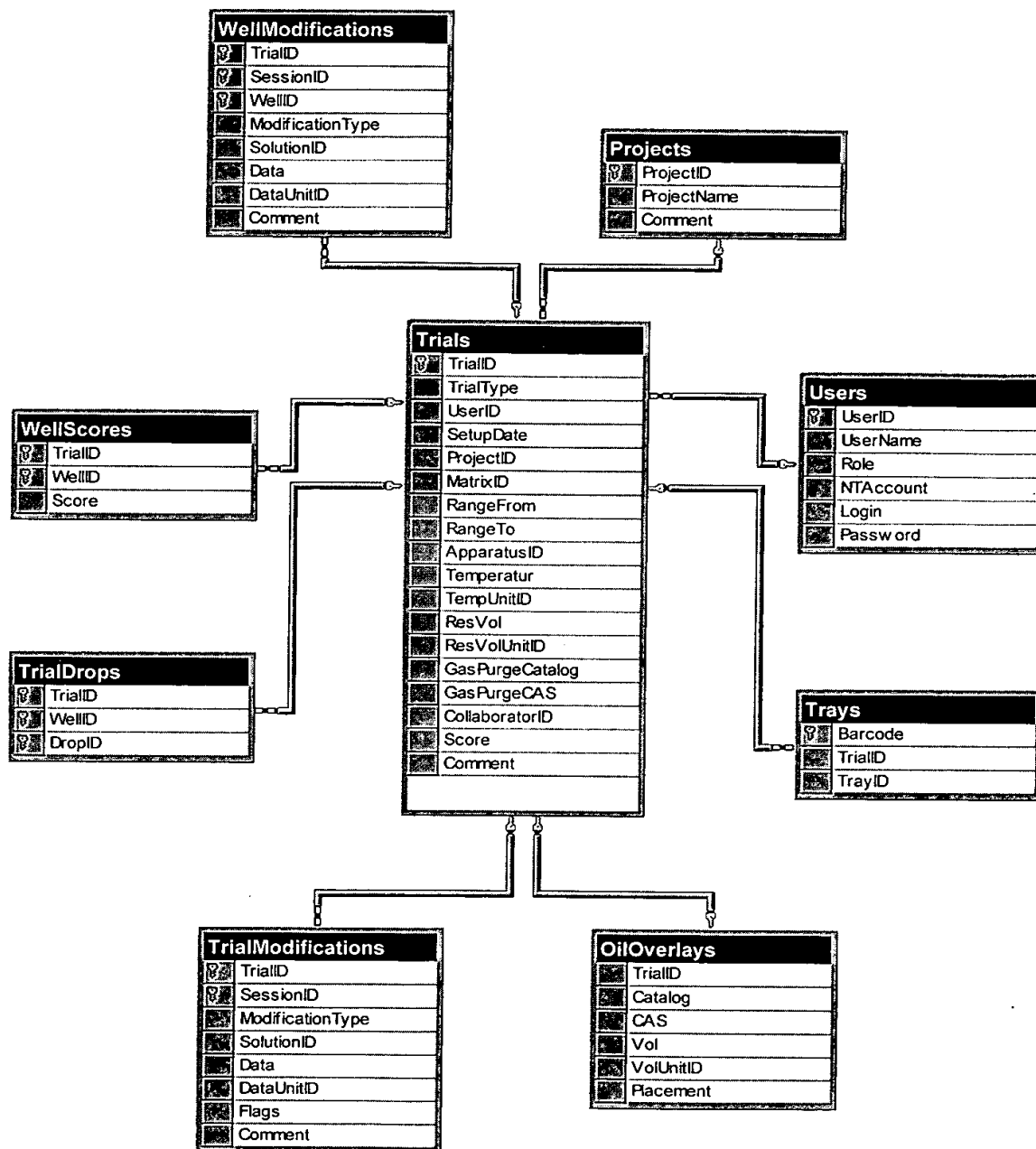
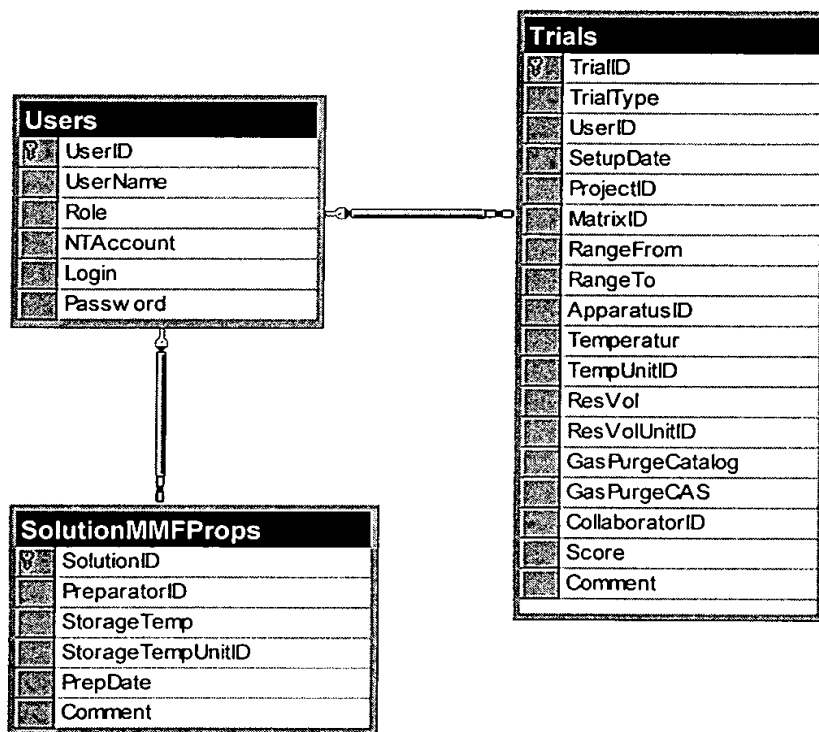


Fig. 260

002080-587E960



**Fig. 261**

002280 - 58T8960

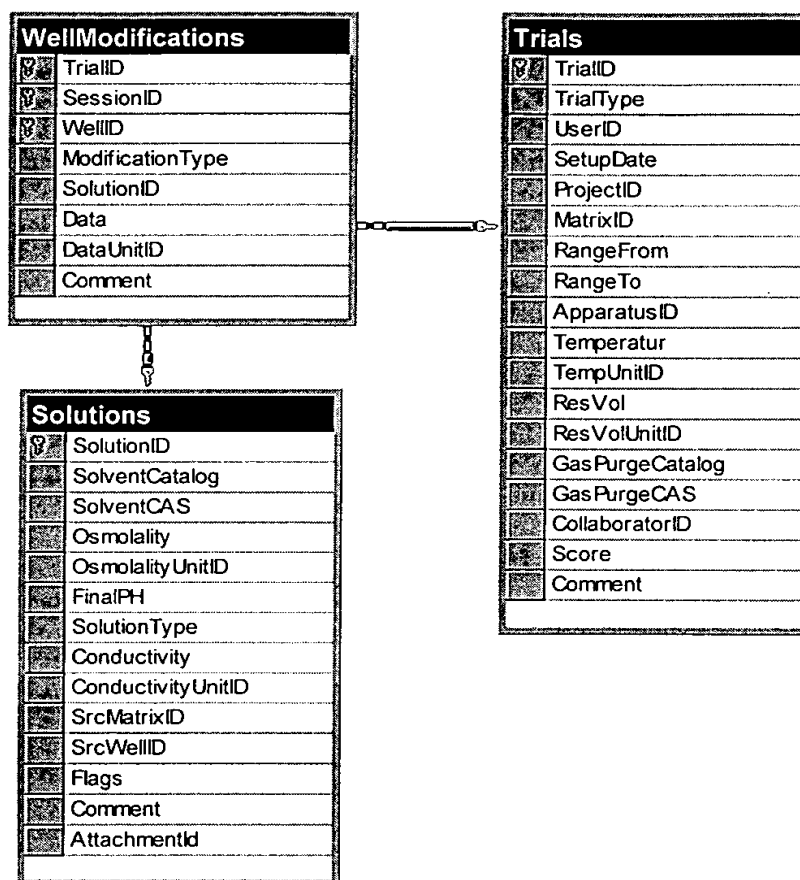
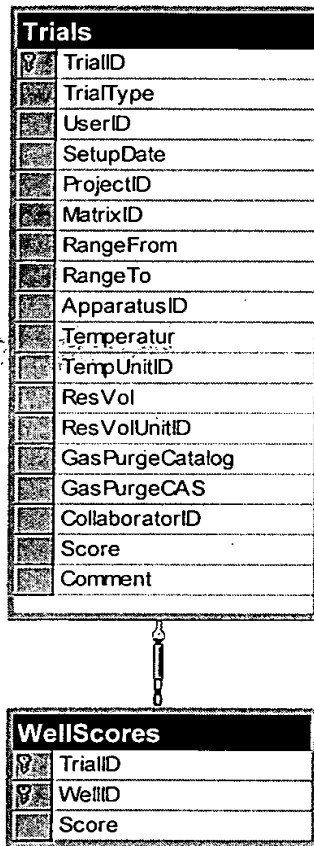


Fig. 262

002030" SBTTC950



**Fig. 263**